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L33 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN

APPLICANT

AN 2004:287803 HCAPLUS
DN 140:310272
ED Entered STN: 08 Apr 2004
TI Process for the hydroformylation of an ethylenically unsaturated compound
IN **Drent, Eit; Van Ginkel, Roelof; Jager, Willem Wabe**
PA Shell Internationale Research Maatschappij B.V., Neth.
SO PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM B01J-0031/24
ICS B01J-0027/08; B01J-0031/02; C07F-0009/6568; C07F-0015/00; C07C-0045/50
CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)
Section cross-reference(s): 23
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004028689	A2	20040408	2003WO-EP50654	20030924 <--
WO2004028689	A3	20040729		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA---2500095	AA	20040408	2003CA-2500095	20030924 <--
AU2003299066	A1	20040419	2003AU-0299066	20030924 <--
US2004167362	A1	20040826	2003US-0670105	20030924 <--
EP---1542798	A2	20050622	2003EP-0798198	20030924 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN---1684769	A	20051019	2003CN-0823006	20030924 <--
JP2006500415	T2	20060105	2004JP-0539074	20030924 <--
ZA2005002080	A	20050912	2005ZA-0002080	20050311 <--
PRAI 2002EP-0256696	A	20020926 <--		
2003WO-EP50654	W	20030924		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004028689	ICM	B01J-0031/24
	ICS	B01J-0027/08; B01J-0031/02; C07F-0009/6568; C07F-0015/00; C07C-0045/50
	IPCI	B01J0031-24 [ICM,7]; B01J0031-16 [ICM,7,C*]; B01J0027-08 [ICS,7]; B01J0027-06 [ICS,7,C*]; B01J0031-02 [ICS,7]; C07F0009-6568 [ICS,7]; C07F0009-00 [ICS,7,C*]; C07F0015-00 [ICS,7]; C07C0045-50 [ICS,7]; C07C0045-00 [ICS,7,C*]
	IPCR	B01J0031-16 [I,C*]; B01J0031-24 [I,A]; B01J0031-26

noble jarrell 10/08/2006

		[N,C*]; B01J0031-28 [N,A]; C07C0045-00 [I,C*]; C07C0045-50 [I,A]; C07C0067-00 [I,C*]; C07C0067-347 [I,A]; C07F0009-00 [I,C*]; C07F0009-6568 [I,A]
	ECLA	B01J031/24; C07C045/50; C07C067/347+69/716; C07C067/347+69/675; C07F009/6568C
CA---2500095	IPCI	B01J0031-24 [ICM,7]; B01J0031-16 [ICM,7,C*]; C07F0015-00 [ICS,7]; B01J0031-02 [ICS,7]; B01J0027-08 [ICS,7]; B01J0027-06 [ICS,7,C*]; C07C0045-50 [ICS,7]; C07C0045-00 [ICS,7,C*]; C07F0009-6568 [ICS,7]; C07F0009-00 [ICS,7,C*]
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US2004167362	IPCI	C07C0045-49 [ICM,7]; C07C0045-00 [ICM,7,C*]
	IPCR	B01J0031-16 [I,C*]; B01J0031-24 [I,A]; B01J0031-26 [N,C*]; B01J0031-28 [N,A]; C07C0045-00 [I,C*]; C07C0045-50 [I,A]; C07C0067-00 [I,C*]; C07C0067-347 [I,A]; C07F0009-00 [I,C*]; C07F0009-6568 [I,A]
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	ECLA	B01J031/24; C07C045/50; C07C067/347+69/675; C07C067/347+69/716; C07F009/6568C
EP---1542798	IPCI	B01J0031-24 [ICM,7]; B01J0031-16 [ICM,7,C*]; B01J0027-08 [ICS,7]; B01J0027-06 [ICS,7,C*]; B01J0031-02 [ICS,7]; C07F0009-6568 [ICS,7]; C07F0009-00 [ICS,7,C*]; C07F0015-00 [ICS,7]; C07C0045-50 [ICS,7]; C07C0045-00 [ICS,7,C*]
	IPCR	B01J0027-06 [I,C*]; B01J0027-08 [I,A]; B01J0031-02 [I,A]; B01J0031-02 [I,C*]; B01J0031-16 [I,C*]; B01J0031-24 [I,A]; C07C0045-00 [I,C*]; C07C0045-50 [I,A]; C07F0009-00 [I,C*]; C07F0009-6568 [I,A]; C07F0015-00 [I,A]; C07F0015-00 [I,C*]
CN---1684769	IPCI	B01J0031-24 [ICM,7]; B01J0031-16 [ICM,7,C*]; B01J0027-08 [ICS,7]; B01J0027-06 [ICS,7,C*]; B01J0031-02 [ICS,7]; C07F0009-6568 [ICS,7]; C07F0009-00 [ICS,7,C*]; C07F0015-00 [ICS,7]; C07C0045-50 [ICS,7]; C07C0045-00 [ICS,7,C*]
	IPCR	B01J0031-16 [I,C*]; B01J0031-24 [I,A]; B01J0031-26 [N,C*]; B01J0031-28 [N,A]; C07C0045-00 [I,C*]; C07C0045-50 [I,A]; C07C0067-00 [I,C*]; C07C0067-347 [I,A]; C07F0009-00 [I,C*]; C07F0009-6568 [I,A]
JP2006500415	IPCI	C07C0067-38 [I,A]; C07C0067-00 [I,C*]; B01J0031-24 [I,A]; B01J0031-16 [I,C*]; C07C0069-675 [I,A]; C07C0069-00 [I,C*]; C07B0061-00 [N,A]
	FTERM	4G169/AA06; 4G169/AA08; 4G169/BA27A; 4G169/BA27B; 4G169/BC69A; 4G169/BC72A; 4G169/BC72B; 4G169/BE26A; 4G169/BE26B; 4G169/BE37A; 4G169/BE37B; 4G169/CB51; 4G169/FA01; 4H006/AA02; 4H006/AC48; 4H006/BA25; 4H006/BA35; 4H006/BA44; 4H006/BA47; 4H006/BA81; 4H006/BE20; 4H006/BE40; 4H006/BN10; 4H006/BT12; 4H039/CC30; 4H039/CL45
ZA2005002080	IPCI	B01J [ICS,7]; C07C [ICS,7]; C07F [ICS,7]
	IPCR	B01J0031-16 [I,C*]; B01J0031-26 [N,C*]; C07C0045-00 [I,C*]; C07C0067-00 [I,C*]; C07F0009-00 [I,C*]; B01J0031-24 [I,A]; B01J0031-28 [N,A]; C07C0045-50

[I,A]; C07C0067-347 [I,A]; C07F0009-6568 [I,A]
ECLA B01J031/24; C07C045/50; C07C067/347+69/675; C07C067/347+69/716; C07F009/6568C

OS MARPAT 140:310272

AB The present invention relates to a process for the hydroformylation of an optionally substituted ethylenically unsatd. compound by reaction thereof with carbon monoxide and hydrogen in the presence of a specific catalyst system. The specific catalyst system comprises (A) a source of group VIII metal cations, (B) a diphosphine ligand having the general formula X1RX2, (C) an acid with pKa < 3, measured in an aqueous solution at 18° or a salt derived thereof, and (D) a source of halide anions, wherein X1, X2 = independently an optionally substituted cyclic group with ≥5 ring atoms, of which one is a phosphorus atom, and R = a bivalent optionally substituted bridging group, connected to each phosphorus atom by a sp2 hybridized carbon atom. Furthermore some specific bidentate diphosphines used in this process are described. Thus, 1,2-dibromobenzene 9.44, 1,4-diazabicyclo[2,2,2]octane 22.4, 9-phosphabicyclo[3.3.1]nonane 13.0, and tetrakis(triphenylphosphine)palladium 2.32 g were heated at 140° to give 7.10 g (yield 50%) 1,2-bis(9-phosphabicyclo[3.3.1]nonyl)benzene, 0.40 mmol of which was mixed with methane sulfonic acid 1.0, hydrochloric acid 0.20, and palladium acetate 0.25 mmol, and 20 mL 1-octene and heated at 120° for 5 h under 20 bar carbon monoxide and 40 bar hydrogen to give an alkanol product >99, a linear alkanol product 68, and a hydrogenation product <1%.

ST process hydroformylation ethylenically unsatd compd; bisphosphabicyclononylbenzene ligand palladium acetate catalyst octene hydroformylation

IT **Alkenes, reactions**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(C11-12; hydroformylation of ethylenically unsatd. compds.)

IT **Ligands**
RL: CAT (Catalyst use); USES (Uses)
(**bidentate, diphosphines**, hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)

IT **Hydroformylation**
(hydroformylation of ethylenically unsatd. compds.)

IT **Group VIII elements**
RL: CAT (Catalyst use); USES (Uses)
(hydroformylation of ethylenically unsatd. compds.)

IT Catalysts
(hydroformylation; hydroformylation of ethylenically unsatd. compds.)

IT **676992-18-0 676992-19-1**
RL: CAT (Catalyst use); USES (Uses)
(hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)

IT **407578-79-4P**, 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(1,2-phenylene)bis- **676992-15-7P** **676992-16-8P**
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)

IT **3375-31-3**
RL: CAT (Catalyst use); USES (Uses)
(hydroformylation of ethylenically unsatd. compds.)

IT 4547-43-7P, Hexanoic acid, 6-hydroxy-, methyl ester 167707-57-5P, Pentanoic acid, 5-hydroxy-4-methyl-, methyl ester **676992-17-9P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(hydroformylation of ethylenically unsatd. compds.)

IT **111-66-0**, 1-Octene 630-08-0, Carbon monoxide, reactions 818-59-7 1333-74-0, Hydrogen, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(hydroformylation of ethylenically unsatd. compds.)

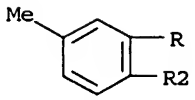
IT 583-53-9, 1,2-Dibromobenzene 3141-26-2, 3,4-Dibromothiophene 13887-02-0, 9-Phosphabicyclo[3.3.1]nonane 75415-78-0, 1,2-Dibromocyclopentene
RL: RCT (Reactant); RACT (Reactant or reagent)

(reactant in hydroformylation catalyst ligand preparation; hydroformylation of ethylenically unsatd. compds.)

IT 676992-18-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydroformylation catalyst ligand; hydroformylation of ethylenically unsatd. compds.)

RN 676992-18-0 HCAPLUS

CN 9-Phosphabicyclo[3.3.1]nonane, 9,9'-(4-methyl-1,2-phenylene)bis- (9CI) (CA INDEX NAME)



L33 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:295834 HCAPLUS

DN 137:108974

ED Entered STN: 21 Apr 2002

TI Teaching a palladium polymerization catalyst to mono-oxygenate olefins

AU Drent, E.; Mul, W. P.; Budzelaar, P. H. M.

CS Shell Research and Technology Centre, Amsterdam, Amsterdam, Neth.

SO Comments on Inorganic Chemistry (2002), 23(2), 127-147
CODEN: COICDZ; ISSN: 0260-3594

PB Taylor & Francis Ltd.

DT Journal

LA English

CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 51, 67

OS CASREACT 137:108974

AB Catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions are efficient catalysts for the hydrocarbonylation of olefins. With these catalyst systems, the oxo-synthesis can be fully exploited to produce, at will, aldehydes/alcs. by hydroformylation or monoketones by hydro-acylation of olefins. The reactions described here constitute the first examples of selective formation of ketones by hydrocarbonylation of higher olefins and the first examples of Pd catalyzed hydroformylation of olefins. Variation of ligand, anion and/or solvent can be used to steer the reaction selectively towards aldehydes/ alcs., ketones or oligoketones. Non-coordinating anions and arylphosphine ligands produce primarily (oligo)ketones; increasing ligand basicity shifts selectivity towards monoketones, while increasing ligand basicity and/or increasing anion coordination strength leads to high selectivity for hydroformylation products, aldehydes and alcs. For the mechanisms of the aldehyde-producing step, we propose protonation of Pd(II)-acyl intermediates, assisted by the coordination of the anion, followed by reductive elimination of the aldehyde and heterolytic dihydrogen cleavage. For selective saturated monoketone formation we propose protonation at the Pd(II)-alkyl stage, now assisted by

chelating carbonyl coordination followed by reductive elimination of the ketone and heterolytic dihydrogen cleavage. Unsatd. ketone formation involves β-hydride elimination from the same Pd(II)-alkyl intermediates.

ST olefin hydrocarbonylation hydroformylation palladium catalyst

IT **Ligands**
RL: CAT (Catalyst use); USES (Uses)
(**bidentate** phosphines; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) **diphosphine** complex with weakly or non-coordinating counterions)

IT Alcohols, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation under hydroformylation conditions; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Addition reaction
Hydroaddition reaction catalysts
(hydroacylation; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT **Hydroformylation**
Hydroformylation catalysts
Regiochemistry
Solvent effect
(hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT **Alkenes, reactions**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); **RCT (Reactant)**; PROC (Process); **RACT (Reactant or reagent)**
(hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Aldehydes, preparation
Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Chemoselectivity
(hydroformylation vs. hydroacylation; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Anions
(ligand/anion effects on catalysis; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Steric effects
(of phosphine ligand; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Carbonylation
Carbonylation catalysts
(reductive; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Synthesis gas
(selective production of ketones or aldehydes at will from olefins and syngas; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)

IT Ketones, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(α,β-unsatd.; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly

or non-coordinating counterions)
IT 76-05-1, Trifluoroacetic acid, uses 104-15-4, p-Toluenesulfonic acid, uses 1493-13-6, Trifluoromethanesulfonic acid
RL: CAT (Catalyst use); USES (Uses)
(anion precursor; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)
IT 3375-31-3, Palladium diacetate
RL: CAT (Catalyst use); USES (Uses)
(catalyst precursor; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)
IT 78-84-2P, Isobutyraldehyde 7786-29-0P, α-Methyloctanal 27644-47-9P, α-Propylhexanal 27649-40-7P, α-Ethylheptanal
RL: BYP (Byproduct); PREP (Preparation)
(hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)
IT 111-66-0, 1-Octene 115-07-1, Propene, reactions
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)
IT 123-72-8P, Butanal 124-19-6P, Nonanal 7379-12-6P, 2-Methyl-3-hexanone 53252-19-0P, 2-Methyl-4-hexen-3-one 62834-80-4P, 2-Methyl-1-hexen-3-one
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)
IT 6737-42-4, 1,3-Bis(diphenylphosphino)propane 121115-33-1, 1,3-Bis(di-tert-butylphosphino)propane 131285-34-2, 1,3-Bis(dibutylphosphino)propane 143540-35-6, 1,3-Bis(di-sec-butylphosphino)propane 159460-98-7, 1,2-Bis(di-sec-butylphosphino)ethane
RL: CAT (Catalyst use); USES (Uses)
(ligand; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly or non-coordinating counterions)
RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Cornils, B; Hydroformylation, Oxo Synthesis, Roelen Reaction in New Syntheses with Carbon Monoxide 1980
(2) Dekker, G; J Organomet Chem 1992, V430, P357 HCAPLUS
(3) Drent, E; GB---2183631 1985 HCAPLUS
(4) Drent, E; EP----220767 1985 HCAPLUS
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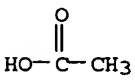
(16) Tolman, C; Chem Rev 1977, V77, P313 HCAPLUS
(17) van Doorn, J; thesis, University of Amsterdam 1991
(18) Zuideveld, M; J Am Chem Soc 1998, V120, P7977 HCAPLUS
IT 3375-31-3, Palladium diacetate
RL: CAT (Catalyst use); USES (Uses); RCT (Reactant); RACT (Reactant or reagent)
(catalyst precursor; hydrocarbonylation of olefins using catalyst systems consisting of a palladium(II) diphosphine complex with weakly

or non-coordinating counterions)
RN 3375-31-3 HCAPLUS
CN Acetic acid, palladium(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Pd(II)

L33 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:851170 HCAPLUS
DN 135:371865
ED Entered STN: 23 Nov 2001
TI Bidentate ligands useful as carbonylation catalysts
IN Drent, Eit; Eberhard, Michael Rolf; Pringle, Paul Gerard
PA Shell Internationale Research Maatschappij BV, Neth.
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07F-0009/50
ICS C07F-0009/6568; C07F-0009/6571; C07C-0045/50; B01J-0031/24
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 45
FAN.CNT 1

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PI	WO2001087899	A1	20011122	2001WO-EP05625	20010516
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	EP---1282629	B1	20040204		
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	ES---2210170	T3	20040701	2001ES-1940491	20010516
	US2002016484	A1	20020207	2001US-0860015	20010517
	US---6639091	B2	20031028		
	ZA2002009309	A	20030729	2002ZA-0009309	20021115
PRAI	2000EP-0304171	A	20000517		
	2001WO-EP05625	W	20010516		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001087899	ICM	C07F-0009/50
	ICS	C07F-0009/6568; C07F-0009/6571; C07C-0045/50; B01J-0031/24
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		B01J0031-24 [ICS,7]; B01J0031-16 [ICS,7,C*]
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US2002016484	IPCI	C07F0009-72 [ICM,7]; C07F0009-90 [ICS,7]; C07F0009-28 [ICS,7]; C07F0009-00 [ICS,7,C*]
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	ECLA	C07C045/50; C07C067/38+69/54; C07C067/38+69/24; C07F009/50A6; C07F009/6568C; C07F009/6571L
ZA2002009309	IPCI	B01J [ICM,7]; C07C [ICS,7]; C07F [ICS,7]

OS CASREACT 135:371865; MARPAT 135:371865

AB The invention describes bidentate ligands of formula R1R2M1-R-M2R3R4, wherein M1 and M2 are independently P, As or Sb; R1, R2, R3 and R4 independently represent tertiary alkyl groups, or R1 and R2 together and/or R3 and R4 together represent an optionally substituted bivalent cycloaliph. group whereby the two free valencies are linked to M1 or M2, and R represents a bivalent aliphatic bridging group containing from 2 to 6 atoms in the bridge, which is substituted with two or more substituents. Use of such a catalyst system in a process for the carbonylation of optionally substituted alkenes and alkynes by reaction with carbon monoxide and a coreactant is described. Thus, propene is hydroformylated by pressurization with carbon monoxide and hydrogen in the presence of

platinum(II) acetylacetonate and meso (R,S) 2,3-[bis(cyclooctylenephosphino)]butane to give 99% n-butyraldehyde.

ST alkene hydroformylation platinum diphosphine cocatalyst; alkanol esterification platinum palladium diphosphine cocatalyst; platinum diphosphine carbonylation cocatalyst; palladium diphosphine carbonylation cocatalyst; aldehyde prepn; ester prepn

IT Alcohols, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aliphatic; esterification of alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

IT **Ligands**
RL: CAT (Catalyst use); USES (Uses)
(**bidentate**; carbonylation reactions of alkenes and alkanols catalyzed by platinum or palladium **diphosphine** cocatalysts)

IT Esterification catalysts
(esterification of alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

IT **Hydroformylation catalysts**
(hydroformylation of alkenes catalyzed by platinum diphosphine cocatalysts)

IT **Alkenes, reactions**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydroformylation of alkenes catalyzed by platinum diphosphine cocatalysts)

IT Esterification
(of alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

IT **Hydroformylation**
(of alkenes catalyzed by platinum diphosphine cocatalysts)

IT **3375-31-3** 15170-57-7, Platinum acetylacetonate 153280-11-6 374557-18-3
RL: CAT (Catalyst use); USES (Uses)
(carbonylation reactions of alkenes and alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

IT 123-72-8P, n-Butyraldehyde 141-32-2P 590-01-2P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(carbonylation reactions of alkenes and alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

IT 71-36-3, Butanol, reactions **74-85-1**, Ethene, reactions 74-86-2, Acetylene, reactions 79-09-4, Propionic acid, reactions **115-07-1**, Propene, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(carbonylation reactions of alkenes and alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD

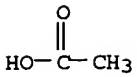
RE

(1) Cyanamid Canada Inc; CA---2086285 A 1994 HCAPLUS
(2) Mason, R; US---3527818 A 1970
(3) Shell Internationale Research Maatschappij BV; EP---0495547 A 1992 HCAPLUS
(4) Shell Internationale Research Maatschappij BV; WO---9505354 A 1995 HCAPLUS
(5) Shell Internationale Research Maatschappij BV; WO---9842717 A 1998 HCAPLUS

IT **3375-31-3**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(carbonylation reactions of alkenes and alkanols catalyzed by platinum or palladium diphosphine cocatalysts)

RN 3375-31-3 HCAPLUS

CN Acetic acid, palladium(2+) salt (8CI, 9CI) (CA INDEX NAME)



●1/2 Pd(II)

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L39 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2006:210242 HCAPLUS
DN 144:254241
TI Novel bis-diazaphospholane ligands for transition-metal catalyzed asymmetric hydroformylation and hydrocyanation
IN Landis, Clark R.; Clark, Thomas P.; Klosin, Jerzy
PA The Dow Chemical Company, USA; Wisconsin Alumni Research Foundation
SO PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2006026489	A1	20060309	2005WO-US30519	20050825
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OS MARPAT 144:254241
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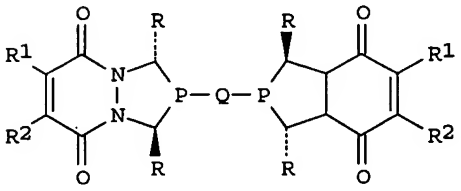


I

AB Novel bis-diazaphospholanes I [Q = optionally substituted alkyl, alkenyl, (hetero)aryl, ferrocenyl; R = carboxy-, carboxamide-, carboxyhydroxamate-alkoxy or amino-substituted (hetero)aryl cycloalkyl, alkyl; R1, R2 = H, (cyclo)alkyl, aryl, or R1-R2 form (un)substituted aryl, cycloalkyl; preferably Q = 1,2-phenylene, R = 2-carboxyphenyl] and their enantiomers were prepared by heterocyclization of diphosphine with azinodimethylidynebis-benzoic acid and phthaloyl or succinyl chloride; the ligands showed high activity and stereoselectivity in rhodium-catalyzed asym. hydroformylation of α-alkenes. In an example, racemic proligand I (1, Q = 1,2-C6H4,

R = 1,2-C6H4COOH, R1-R2 = benzo) was prepared by heterocyclization of 1,2-HOOCC6H4CH:NN:CHC6H4COOH-1,2 with 1,2-C6H4(PH3)2 and phthaloyl chloride with 21% yield; compound 1 was then converted into enantiomerically pure amide (1R,3R)-I [3; R = 1,2-C6H4CONH-(S)-CHMeCO2Me, Q = 1,2-C6H4, R1-R2 = benzo] by reaction with L-alanine Me ester. In another example, ligand 3 was used in asym. hydroformylation fo vinyl acetate, giving (2R)-2-acetoxypropanal with 84% yield, 26.3 branched/linear ratio and 84% ee.

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 28, 45

IT **Hydroformylation catalysts**
(stereoselective; preparation of chiral bis-1,2,4-diazaphospholanes as ligands for rhodium-catalyzed asym. hydroformylation)

IT **Alkenes, reactions**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(α-; preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

IT **851770-13-3P**
RL: CAT (Catalyst use); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

IT **7439-88-5D**, Iridium, complexes **7439-89-6D**, Iron, complexes **7440-02-0D**, Nickel, complexes **7440-04-2D**, Osmium, complexes **7440-05-3D**, Palladium, complexes **7440-06-4D**, Platinum, complexes **7440-16-6D**, Rhodium, complexes **7440-18-8D**, Ruthenium, complexes **7440-48-4D**, Cobalt, complexes
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

IT **851609-32-0P 851609-33-1P 851609-34-2P 851609-35-3P 851609-36-4P 851770-14-4P 851770-15-5P 851770-16-6P 851770-17-7P**
RL: CAT (Catalyst use); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

IT **615257-74-4P 615538-63-1P 877176-11-9P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

IT **851609-30-8P 851609-31-9P 877081-79-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

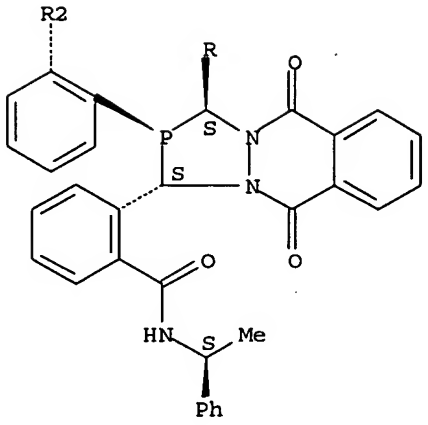
IT **851770-13-3P**
RL: CAT (Catalyst use); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

RN 851770-13-3 HCAPLUS

CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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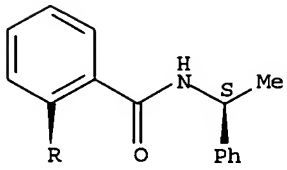

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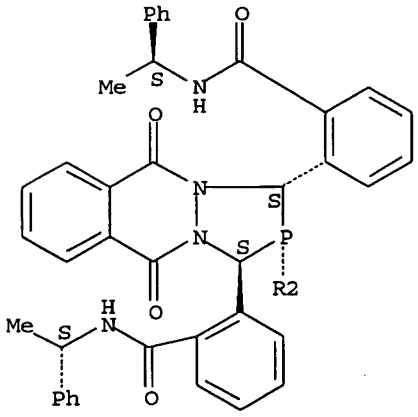


IT 7439-88-5D, Iridium, complexes 7439-89-6D, Iron, complexes 7440-02-0D, Nickel, complexes 7440-04-2D, Osmium, complexes 7440-05-3D, Palladium, complexes 7440-06-4D, Platinum, complexes 7440-16-6D, Rhodium, complexes 7440-18-8D, Ruthenium, complexes 7440-48-4D, Cobalt, complexes
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

RN 7439-88-5 HCAPLUS
CN Iridium (8CI, 9CI) (CA INDEX NAME)

Ir

RN 7439-89-6 HCAPLUS
CN Iron (7CI, 8CI, 9CI) (CA INDEX NAME)

Fe

RN 7440-02-0 HCAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-04-2 HCAPLUS
CN Osmium (8CI, 9CI) (CA INDEX NAME)

Os

RN 7440-05-3 HCAPLUS
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCAPLUS
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

RN 7440-16-6 HCAPLUS
CN Rhodium (8CI, 9CI) (CA INDEX NAME)

Rh

RN 7440-18-8 HCAPLUS
CN Ruthenium (8CI, 9CI) (CA INDEX NAME)

Ru

RN 7440-48-4 HCAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

Co

IT **851609-32-0P 851609-33-1P 851609-34-2P**
851609-35-3P 851609-36-4P 851770-14-4P
851770-15-5P 851770-16-6P 851770-17-7P

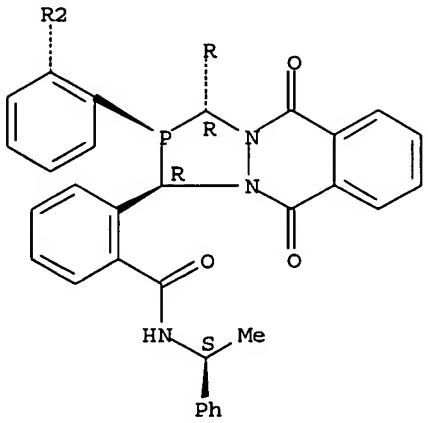
RL: CAT (Catalyst use); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

RN 851609-32-0 HCAPLUS

CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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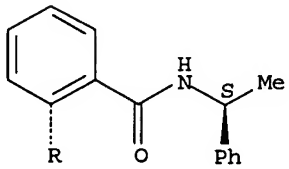

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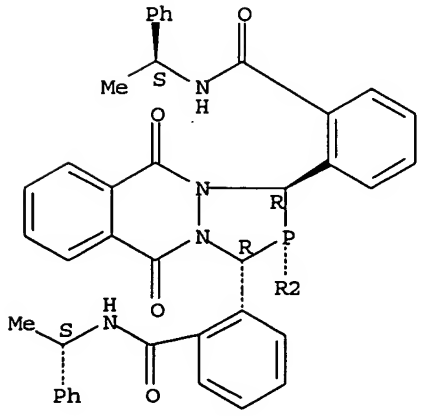
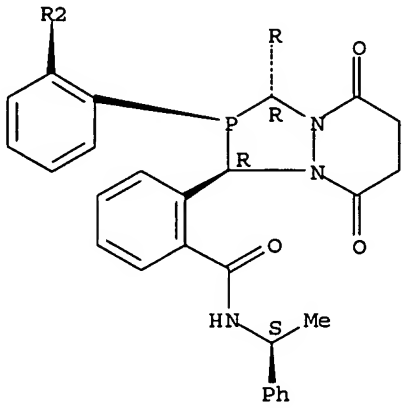


RN 851609-33-1 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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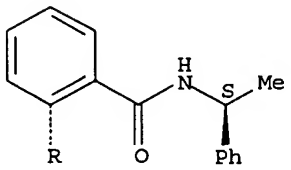

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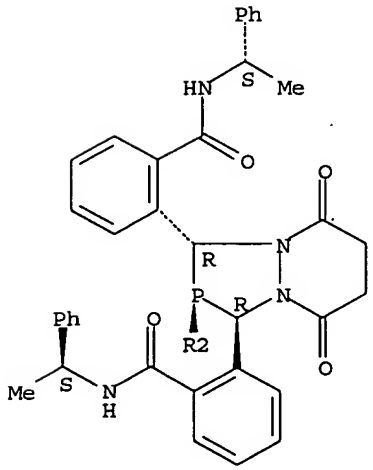
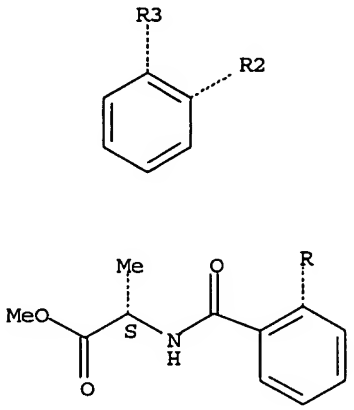


RN 851609-34-2 HCAPLUS

CN L-Alanine, N,N',N'',N'''-[1,2-phenylenebis[(1R,3R)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]bis(2,1-phenylenecarbonyl)]tetrakis-, tetramethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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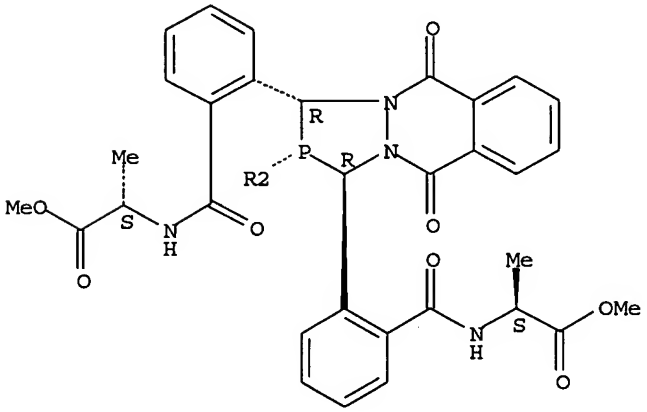

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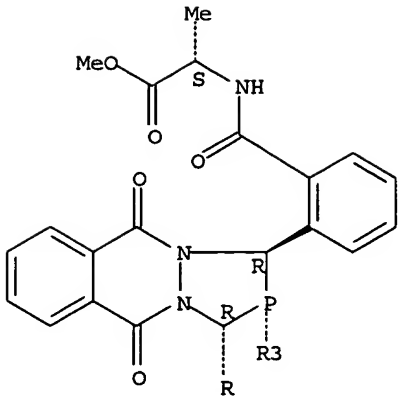

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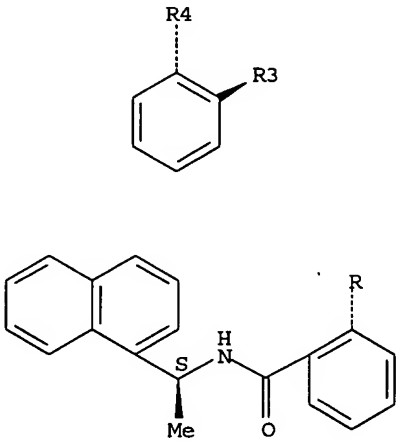
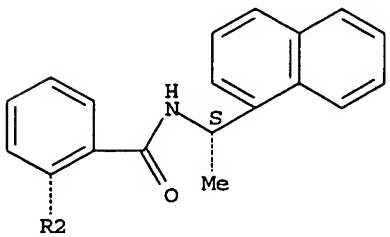
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-(1-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



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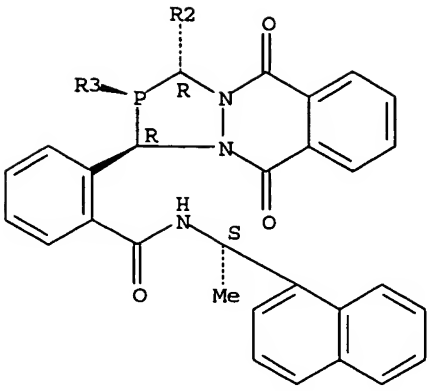

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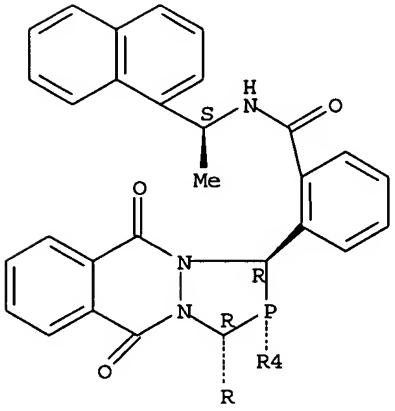
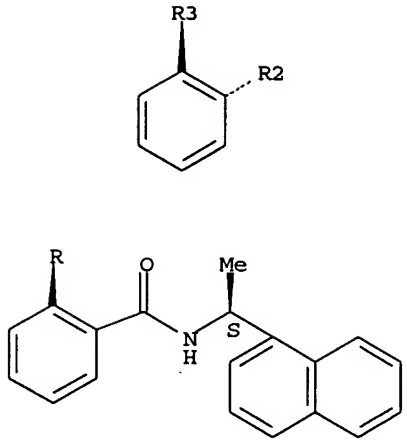


RN 851609-36-4 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-(1-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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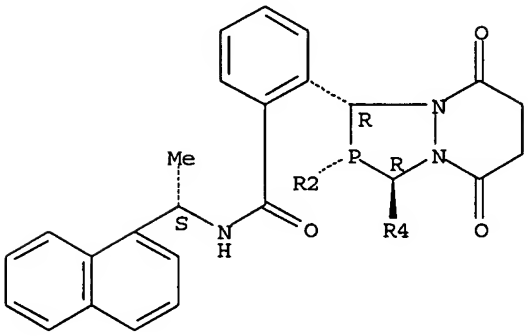

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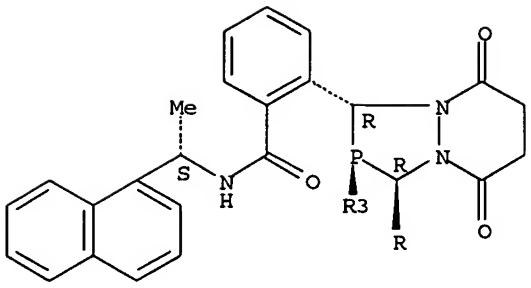
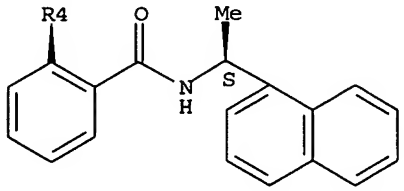
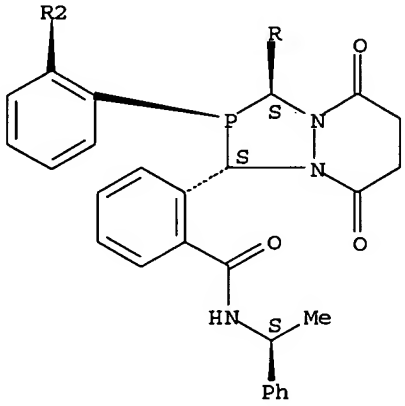




RN 851770-14-4 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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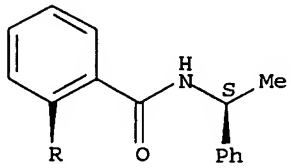

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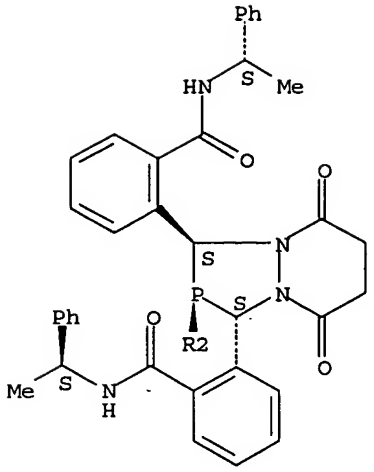
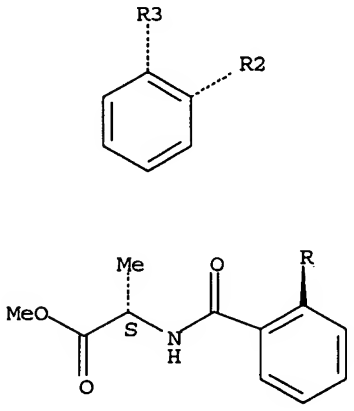


RN 851770-15-5 HCAPLUS
CN L-Alanine, N,N',N'',N'''-[1,2-phenylenebis[[(1S,3S)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]bis(2,1-phenylenecarbonyl)]]tetrakis-, tetramethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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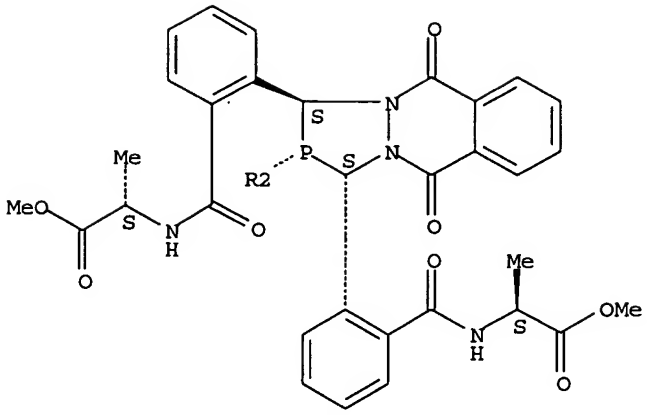

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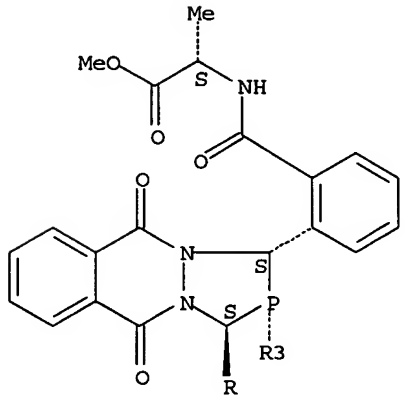
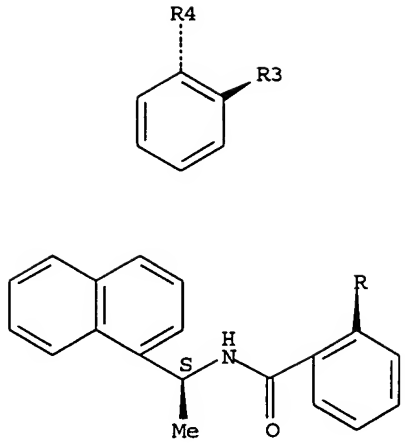


RN 851770-16-6 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-(1-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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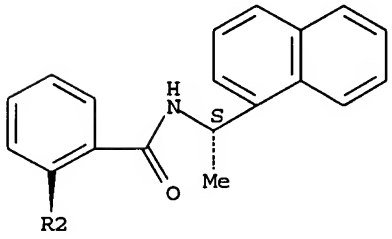

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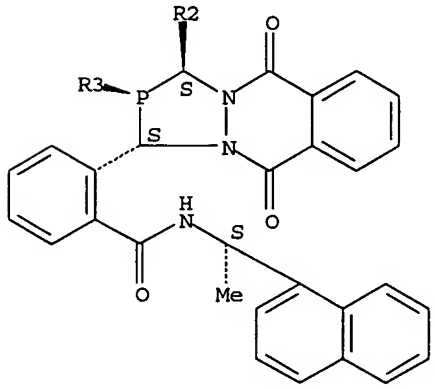
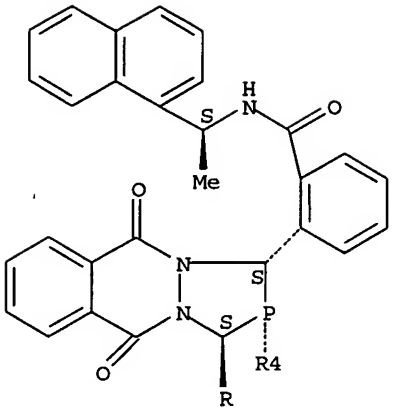


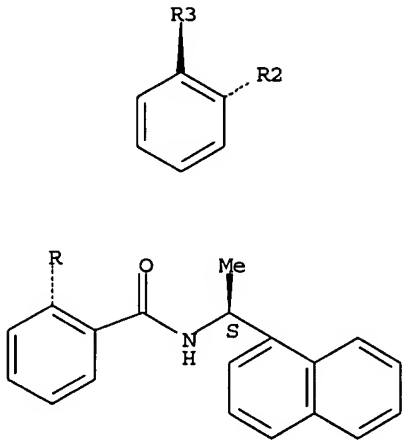
PAGE 4-A



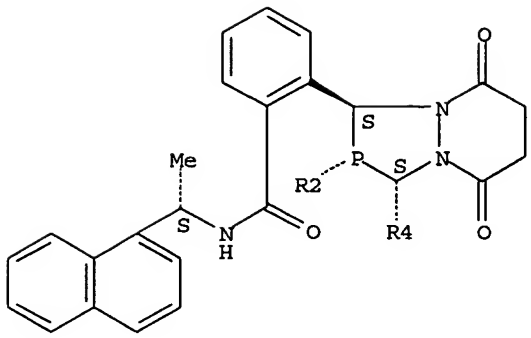
RN 851770-17-7 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-(1-naphthalenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



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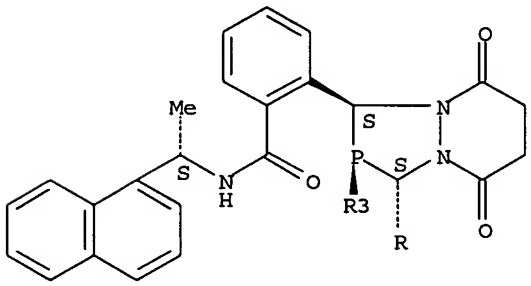
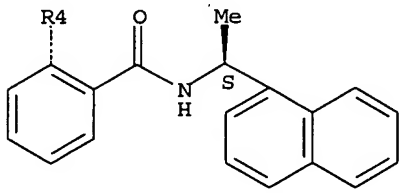




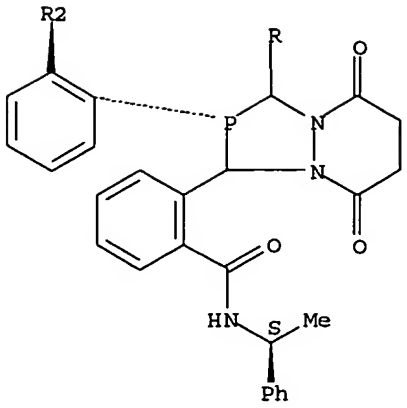
IT 877176-11-9P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

RN 877176-11-9 HCAPLUS

CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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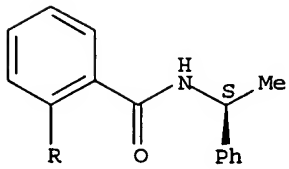

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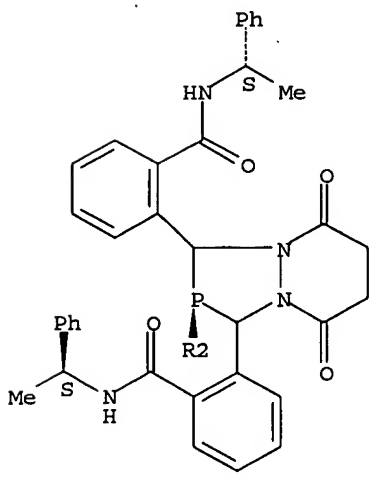


IT 851609-30-8P 851609-31-9P 877081-79-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral bis-1,2,4-diazaphospholane tetrakis-carboxamides as ligands for rhodium-catalyzed asym. hydroformylation)

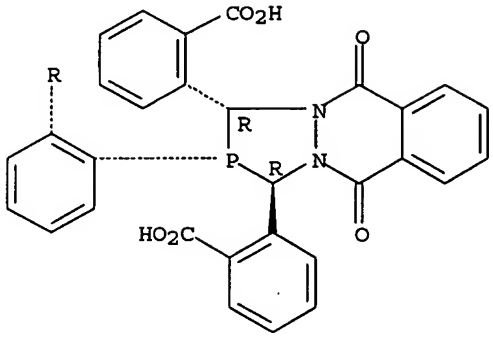
RN 851609-30-8 HCAPLUS

CN Benzoic acid, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis-

, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



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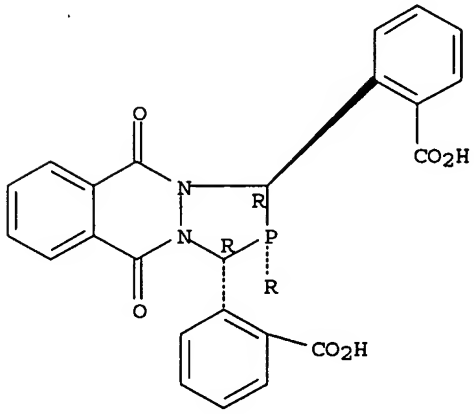
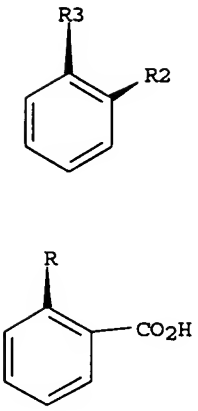


RN 851609-31-9 HCAPLUS
CN Benzoic acid, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



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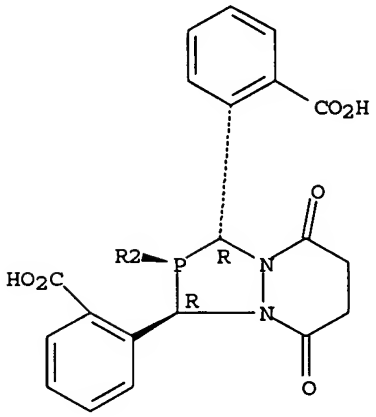

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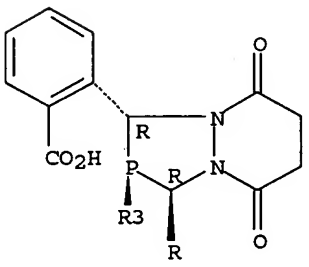
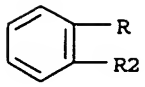
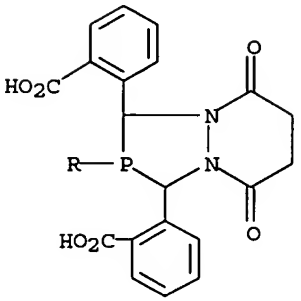


RN 877081-79-3 HCAPLUS
CN Benzoic acid, 2,2',2'',2'''-[1,2-phenylenebis[tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis- (9CI) (CA INDEX NAME)

PAGE 1-A





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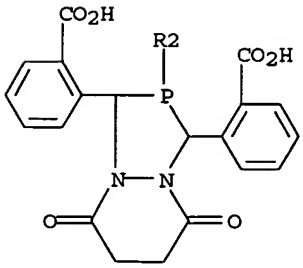

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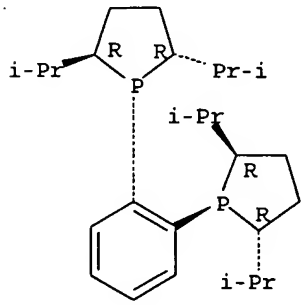
Kwok, T	1993	12	1954	ORGANOMETALLICS	HCAPLUS
Nozaki, K	1997	119	4413	JOURNAL OF THE AMERI	HCAPLUS
Reetz, M	2003			US2003171608 A1	HCAPLUS
The Penn State Research	2003			WO--03042135 A	HCAPLUS
Zhang, X	2003			US2003040629 A1	
Zhang, X	2003			US2003144137 A1	HCAPLUS
Zhang, X	2004			US2004072680 A1	
Zhang, X	2004			US2004229846 A1	

L39 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1084713 HCAPLUS
DN 144:36155
TI A highly enantioselective catalyst for asymmetric hydroformylation of [2.2.1]-bicyclic olefins
AU Huang, Jinkun; Bunel, Emilio; Allgeier, Alan; Tedrow, Jason; Storz, Thomas; Preston, J.; Correll, Tiffany; Manley, Deana; Soukup, Troy; Jensen, Randy; Syed, Rashid; Moniz, George; Larsen, Robert; Martinelli, Michael; Reider, Paul J.
CS Chemical Process Research & Development, Amgen Inc., Thousand Oaks, CA, 91320, USA
SO Tetrahedron Letters (2005), 46(45), 7831-7834
CODEN: TELEAY; ISSN: 0040-4039

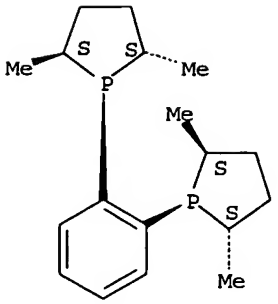
PB Elsevier B.V.
DT Journal
LA English
AB Rh(CO)2(acac)/TangPhos was found to be a highly enantioselective catalyst for asym. hydroformylation of norbornylene under mild conditions. Application of the protocol to the desymmetrization of other [2.2.1]-bicyclic olefins gave moderate to excellent enantioselectivity (55-92% ee).
CC 24-7 (Alicyclic Compounds)
Section cross-reference(s): 28
IT **Cycloalkenes**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(bicyclic; rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos ligand)
IT **Hydroformylation**
Hydroformylation catalysts
(stereoselective; rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos ligand)
IT **136705-65-2 136735-95-0 136779-26-5 136779-27-6 136779-28-7**
RL: CAT (Catalyst use); USES (Uses)
(rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos and related ligands)
IT **14874-82-9**, Rhodium dicarbonyl acetylacetonate **752258-19-8**
RL: CAT (Catalyst use); USES (Uses)
(rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos ligand)
IT 100-42-5, Styrene, reactions 129-64-6 **498-66-8**, Norbornylene 2746-19-2 7213-65-2 39203-22-0 49675-21-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos ligand)
IT **136705-65-2 136735-95-0 136779-28-7**
RL: CAT (Catalyst use); USES (Uses)
(rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos and related ligands)
RN 136705-65-2 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-bis(1-methylethyl)-, (2R,2'R,5R,5'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



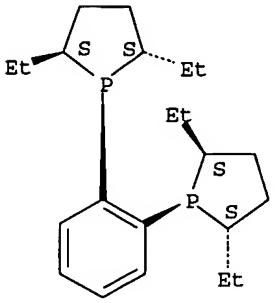
RN 136735-95-0 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-dimethyl-, (2S,2'S,5S,5'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

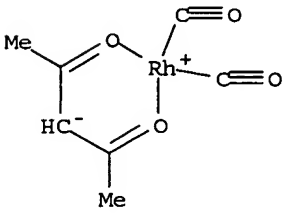


RN 136779-28-7 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-diethyl-, (2S,2'S,5S,5'S)- (9CI) (CA INDEX NAME)

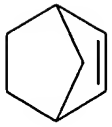
Absolute stereochemistry.



IT **14874-82-9**, Rhodium dicarbonyl acetylacetonate
RL: CAT (Catalyst use); USES (Uses)
(rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos ligand)
RN 14874-82-9 HCAPLUS
CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)- (9CI) (CA INDEX NAME)



IT **498-66-8**, Norbornylene
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(rhodium-catalyzed asym. hydroformylation of [2.2.1]-bicyclic olefins using TangPhos ligand)
RN 498-66-8 HCAPLUS
CN Bicyclo[2.2.1]hept-2-ene (9CI) (CA INDEX NAME)



RETABLE

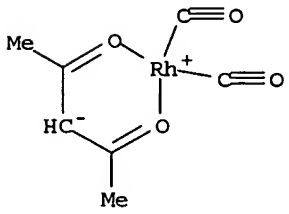
Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Agbossou, F	1995	95	2485	Chem Rev	HCAPLUS
Clark, T	2005	127	5040	J Am Chem Soc	HCAPLUS
Consiglio, G	1991	10	2046	Organometallics	HCAPLUS
Gladiali, S	1995	6	1453	Tetrahedron:Asymmetr	HCAPLUS
Koser, G	2001	34	89	Aldrichim Acta	HCAPLUS
Koser, G	1977	42	1476	J Org Chem	HCAPLUS
Lu, S	2000	63	531	Catal Today	HCAPLUS
Luna, A	2002	124	12098	J Am Chem Soc	
Luna, A	2002	67	3522	J Org Chem	HCAPLUS
Nozaki, K	2001	343	61	Adv Synth Catal	HCAPLUS
Nozaki, K	2000		429	Catalytic Asymmetric	HCAPLUS
Nozaki, K	1997	119	3313	J Am Chem Soc	
Nozaki, K	1998	120	4051	J Am Chem Soc	HCAPLUS
Parrinello, G	1987	109	7122	J Am Chem Soc	HCAPLUS
Parrinello, G	1986	51	4189	J Org Chem	HCAPLUS
Sakai, S	1993	115	7033	J Am Chem Soc	
Tang, W	2002	41	1612	Angew Chem, Int Ed	HCAPLUS

L39 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1056265 HCAPLUS
DN 143:477689
TI Highly regio- and enantioselective asymmetric hydroformylation of olefins mediated by 2,5-disubstituted phospholane ligands
AU Axtell, Alex T.; Cobley, Christopher J.; Klosin, Jerzy; Whiteker, Gregory T.; Zanotti-Gerosa, Antonio; Abboud, Khalil A.
CS Chemical Sciences, The Dow Chemical Company, Midland, MI, 48674, USA
SO Angewandte Chemie, International Edition (2005), 44(36), 5834-5838
CODEN: ACIEF5; ISSN: 1433-7851
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
OS CASREACT 143:477689
AB The com. available ligand (R,R)-1,2-bis(2,5-diphenylphospholano)ethane [(R,R)-Ph-bpe] has been identified as an excellent ligand for asym. hydroformylation. State-of-the-art regio- and enantioselectivities are obtained for reactions with styrene, allyl cyanide, and vinyl acetate as substrates while high reaction rates (> 4000 turnovers h-1) are maintained.
CC 25-15 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 23
IT **Alkenes, reactions**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(regio- and stereoselective hydroformylation of olefins mediated by 2,5-disubstituted phospholane ligands)
IT **Hydroformylation**
Hydroformylation catalysts
(regioselective; regio- and stereoselective hydroformylation of olefins mediated by 2,5-disubstituted phospholane ligands)
IT **Hydroformylation**
Hydroformylation catalysts
(stereoselective; regio- and stereoselective hydroformylation of olefins mediated by 2,5-disubstituted phospholane ligands)

IT 14874-82-9, Dicarbonylrhodium acetylacetonate 136705-63-0
136705-64-1, (R,R)Ethyl-duphos 136779-27-6 137151-97-4
147253-67-6, (R,R)Methyl-duphos 147253-69-8
149646-83-3, (R,R)-Chiraphite 149917-85-1, (R,S)-Binaphos 224057-13-0
268541-06-6 528565-79-9 528854-34-4 729572-33-2, (S,S)-Kelliphite
849950-54-5 851770-14-4
RL: CAT (Catalyst use); USES (Uses)
(regio- and stereoselective hydroformylation of olefins mediated by 2,5-disubstituted phospholane ligands)

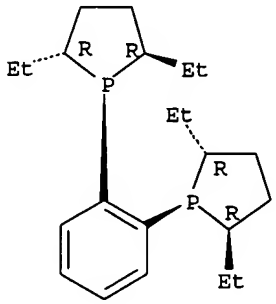
IT 14874-82-9, Dicarbonylrhodium acetylacetonate 136705-64-1
, (R,R)Ethyl-duphos 147253-67-6, (R,R)Methyl-duphos
147253-69-8 851770-14-4
RL: CAT (Catalyst use); USES (Uses)
(regio- and stereoselective hydroformylation of olefins mediated by 2,5-disubstituted phospholane ligands)

RN 14874-82-9 HCAPLUS
CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)- (9CI) (CA INDEX NAME)



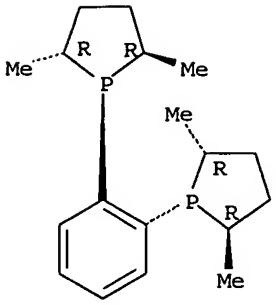
RN 136705-64-1 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-diethyl-, (2R,2'R,5R,5'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



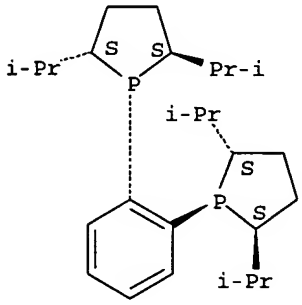
RN 147253-67-6 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-dimethyl-, [2R-[1(2'R*,5'R*),2α,5β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 147253-69-8 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-bis(1-methylethyl)-, [2S-[1(2'R*,5'R*),2α,5β]]- (9CI) (CA INDEX NAME)

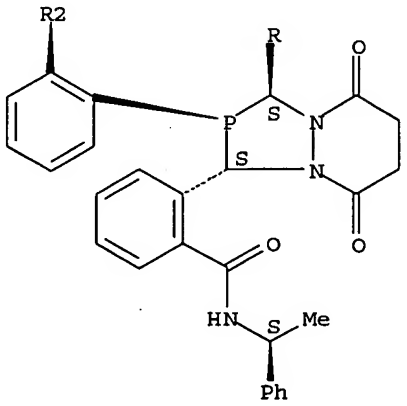
Absolute stereochemistry.



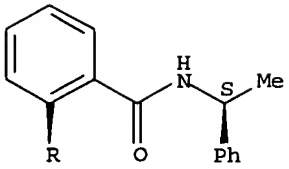
RN 851770-14-4 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

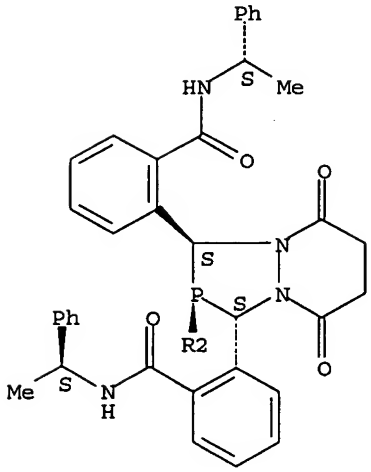
PAGE 1-A



PAGE 2-A



PAGE 3-A



RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Babin, J	1993			WO---9303839	HCAPLUS
Berens, U	2000	112	2057	Angew Chem	
Berens, U	2000	39	1981	Angew Chem Int Ed	HCAPLUS
Breeden, S	2000	112	4272	Angew Chem	
Breeden, S	2000	39	4106	Angew Chem Int Ed	HCAPLUS
Burk, M	2000	33	363	Acc Chem Res	HCAPLUS
Burk, M	1993	115	10125	J Am Chem Soc	HCAPLUS
Cambridge Crystallograp				www.ccdc.cam.ac.uk/d	
Clark, T	2005	127	5040	J Am Chem Soc	HCAPLUS
Claver, C	2000			Rhodium Catalyzed Hy	
Cobley, C	2004	69	4031	J Org Chem	HCAPLUS
Cobley, C	2004	6	3277	Org Lett	HCAPLUS
Cobley, C	2003	7	407	Org Process Res Dev	HCAPLUS
Dieguez, M	2001	7	3086	Chem Eur J	HCAPLUS
Dieguez, M	2004	15	2113	Tetrahedron:Asymmetr	HCAPLUS
Ernst, M	1989	28	1624	Inorg Chem	HCAPLUS
Marinetti, A	1999	12	1975	Synlett	
Moloy, K	1995	117	7696	J Am Chem Soc	HCAPLUS
Mukerjee, S	1988	27	81	Inorg Chem	HCAPLUS
Nozaki, K	1997	119	4413	J Am Chem Soc	HCAPLUS
Pilkington, C	2003	5	1273	Org Lett	HCAPLUS
Stille, J	1991	4	913	Comprehensive Organi	
Tang, W	2003	103	3029	Chem Rev	HCAPLUS
van Leeuwen, P	2000		63	Rhodium Catalyzed Hy	HCAPLUS
van Rooy, A	1995	14	34	Organometallics	HCAPLUS
Whiteker, G	2003	89	359	Chemical Industries	HCAPLUS

L39 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:409532 HCAPLUS
DN 142:463874
TI Preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis
IN Landis, Clark R.; Jin, Wiechang; Owen, Jonathan S.; Clark, Thomas P.; Nelson, Ryan C.
PA Wisconsin Alumni Research Foundation, USA
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2005042546	A2	20050512	2004WO-US25420	20040806
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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OS MARPAT 142:463874
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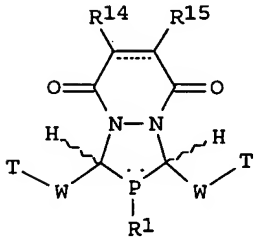


I

AB Preparation of diazaphosphacycles I (W = aryl, cycloalkyl, heterocyclyl, etc.; T = alkoxycarbonyl, aminocarbonyl, alkoxyaminocarbonyl (un)substituted oxazole, etc.; R1 = (un)substituted aryl, alkyl, alkenyl, cycloalkyl, ferrocenyl, etc.; R14, R15 = H, (un)substituted alkyl, cycloalkyl, aryl, etc.; R14R15 = ring) and their salts are provided. Transition metal catalysts incorporating such diazaphosphacycles and methods of use thereof are also disclosed. There are further provided compns. comprising diazaphosphacycles covalently attached to a solid support and methods of use thereof.
IC ICM C07F
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21, 34
IT **Alkenes, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)

(dehydrogenation; preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)

IT Cross-coupling reaction catalysts
Cyclopropanation catalysts
Dehydrogenation catalysts
Hydroboration catalysts
Hydrocyanation catalysts
Hydroformylation catalysts
Hydrosilylation catalysts
Organic synthesis
Solid phase synthesis supports
(preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)

IT **381721-79-5P** 381721-81-9P 381721-85-3P 381721-87-5P 381721-92-2P **381721-98-8P**
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)

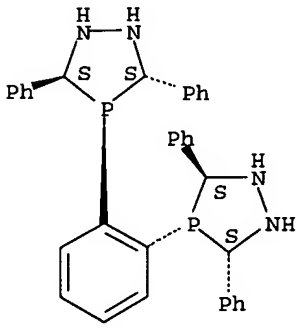
IT 12012-95-2 **12257-42-0** 12266-92-1 35138-22-8
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)

IT 381721-65-9P 381721-66-0P 381721-67-1P 381721-71-7P 381721-73-9P
381721-75-1P 381721-76-2P 381721-88-6P 381721-90-0P 381721-94-4P
381721-96-6P **381722-00-5P** 381722-02-7P 381722-04-9P
494837-78-4P 494837-79-5P 494837-80-8P 494837-83-1P 494837-84-2P
494837-86-4P 494837-87-5P 494837-89-7P 495401-05-3P 495401-06-4P
495401-07-5P 615257-74-4P 615257-75-5P 615257-76-6P 615257-77-7P
615257-78-8P 615257-79-9P 615257-80-2P 615257-81-3P 615257-82-4P
615257-83-5P 615257-84-6P 615257-85-7P 615257-86-8P 615257-87-9P
615538-60-8P 615538-61-9P 615538-62-0P 615538-63-1P 615538-64-2P
615538-65-3P 851519-22-7P 851519-23-8P 851519-24-9P 851673-55-7P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)

IT **381721-98-8P**
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)

RN 381721-98-8 HCAPLUS
CN 1,2,4-Diazaphospholidine, 4,4'-(1,2-phenylene)bis[3,5-diphenyl-, (3R,3'R,5R,5'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

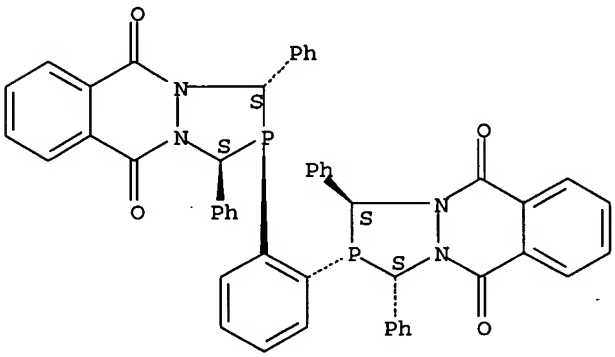


IT **12257-42-0**
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES

(Uses)
(preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)
RN 12257-42-0 HCAPLUS
CN Rhodium, bis[(2,3,5,6-η)-bicyclo[2.2.1]hepta-2,5-diene]di-μ-chlorodi- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
IT 381722-00-5P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of diazaphosphacycles and their use in transition metal catalyzed organic synthesis)
RN 381722-00-5 HCAPLUS
CN 1H-[1,2,4]Diazaphospholo[1,2-b]phthalazine-5,10-dione, 2,2'-(1,2-phenylene)bis[2,3-dihydro-1,3-diphenyl-, (1R,1'R,3R,3'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L39 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:241636 HCAPLUS
DN 142:463810
TI Highly Active, Regioselective, and Enantioselective Hydroformylation with Rh Catalysts Ligated by Bis-3,4-diazaphospholanes
AU Clark, Thomas P.; Landis, Clark R.; Freed, Susan L.; Klosin, Jerzy; Abboud, Khalil A.
CS Department of Chemistry, University of Wisconsin-Madison, Madison, WI, 53706, USA
SO Journal of the American Chemical Society (2005), 127(14), 5040-5042
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 142:463810
AB Azines made by the reaction of hydrazine with ortho-formylbenzoic acid react with 1,2-diphosphinobenzene and either succinyl chloride or phthaloyl chloride in ca. 30% yield to give rac-bis-3,4-diazaphospholanes bearing benzoic acid groups in the 2 and 5 positions. Condensation of the benzoic acid functionalities with enantiomerically pure amines affords diastereomeric benzoamides which can be separated by flash chromatog. The crystal structure of a representative compound is reported. Application of the resolved bis-3,4-diazaphospholanes to Rh-catalyzed enantioselective hydroformylation of styrene, allyl cyanide, and vinyl acetate under mild pressures (20-500 psig of CO/H2) and temps. (40-120 °C) reveals high activities and selectivities for all three substrates. At 60 °C and 500 psig syn gas, the best ligand provides outstanding regio- and enantioselectivities (styrene, 89% ee, b:l = 30:1; allyl cyanide, 87% ee, b:l = 4.8:1; vinyl acetate, 95% ee, b:l = 40:1) while

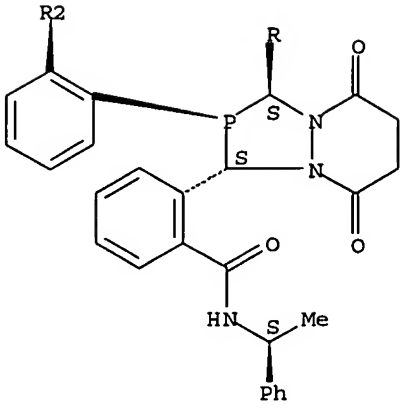
achieving turnover frequencies of ca. 3000 h-1.
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 28, 67, 75
IT **Alkenes, reactions**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
IT **Hydroformylation**
Hydroformylation catalysts
(regioselective, stereoselective; preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed **regioselective and stereoselective** hydroformylation of alkenes)
IT **851770-18-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
IT **851770-14-4P**
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(mol. structure; preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
IT **14874-82-9 149646-83-3 149917-85-1 615257-74-4 729572-33-2**
RL: CAT (Catalyst use); USES (Uses)
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
IT **851609-32-0P 851609-33-1P 851609-34-2P**
851609-35-3P 851609-36-4P 851770-13-3P
851770-15-5P 851770-16-6P 851770-17-7P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
IT **851609-30-8P 851609-31-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
IT **851770-18-8P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(crystal structure; preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
RN 851770-18-8 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]-, compd. with 2-propanone (1:7) (9CI) (CA INDEX NAME)

CM 1

CRN 851770-14-4
CMF C78 H72 N8 O8 P2

Absolute stereochemistry.

PAGE 1-A



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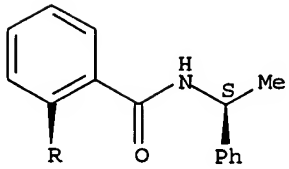

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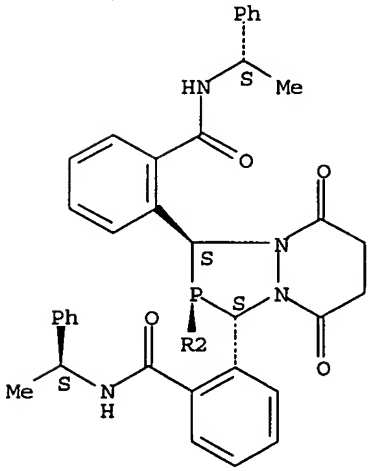
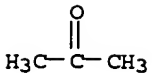


CM 2

CRN 67-64-1
CMF C3 H6 O



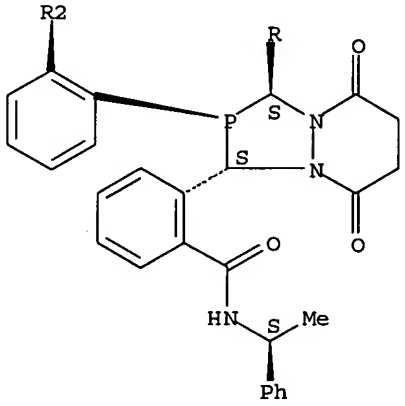
IT **851770-14-4P**
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(mol. structure; preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)

RN 851770-14-4 HCAPLUS

CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1S,3S)-tetrahydro-5,8-dioxo-1H-[1,2,4]diazaphospholo[1,2-a]pyridazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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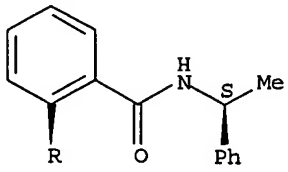

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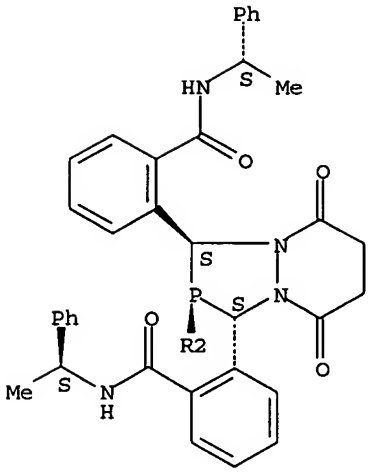

IT 14874-82-9
RL: CAT (Catalyst use); USES (Uses)
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
RN 14874-82-9 HCAPLUS
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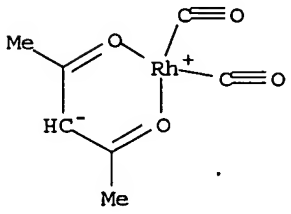

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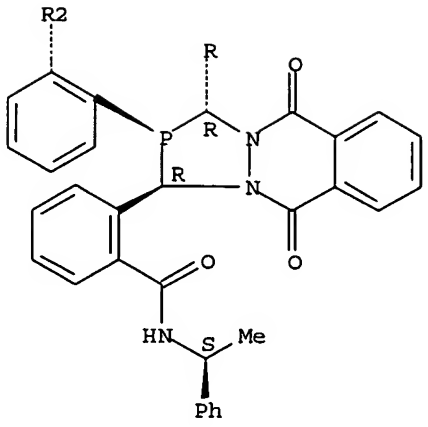
851609-35-3P 851609-36-4P 851770-13-3P
851770-15-5P 851770-16-6P 851770-17-7P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)
RN 851609-32-0 HCAPLUS
CN Benzamide, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis[N-[(1S)-1-phenylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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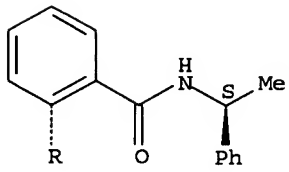

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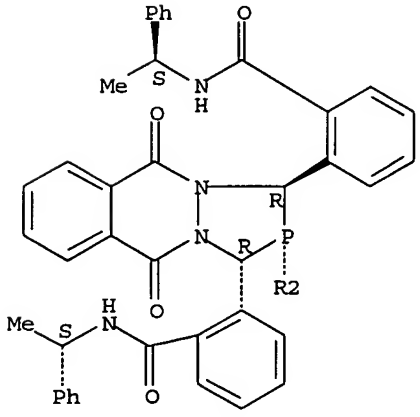

RN 851609-33-1 HCAPLUS
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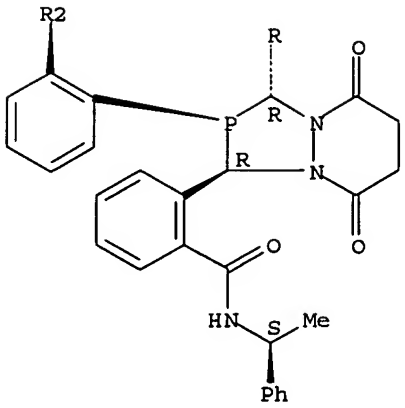
Absolute stereochemistry.

PAGE 1-A



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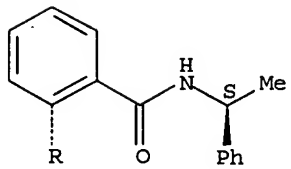

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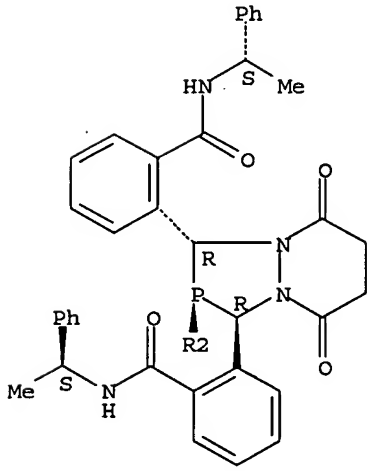

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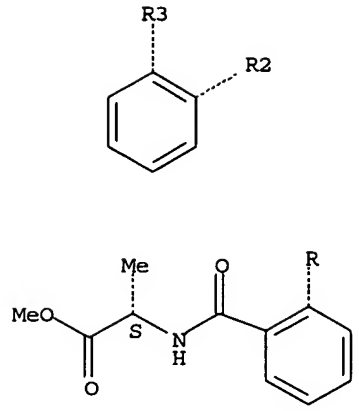
Absolute stereochemistry.

PAGE 1-A



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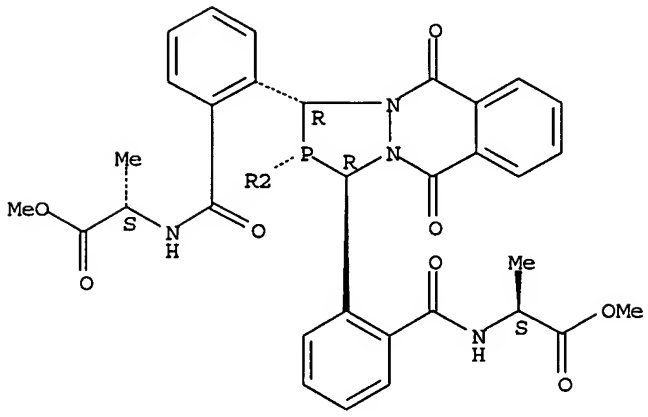

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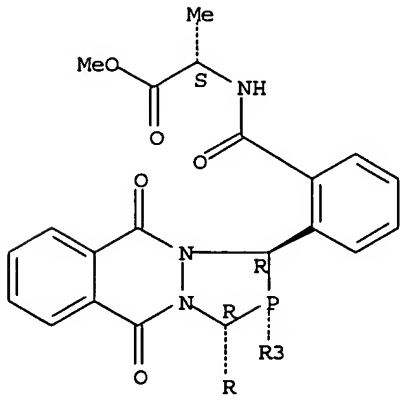

RN 851609-35-3 HCAPLUS

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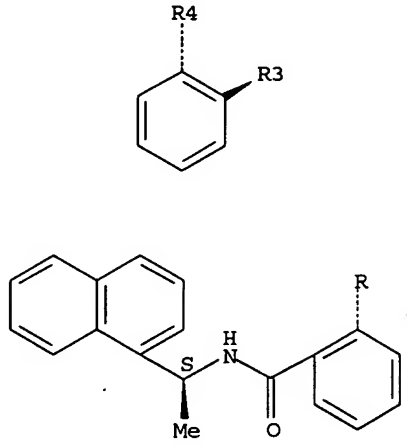
Absolute stereochemistry.

PAGE 1-A



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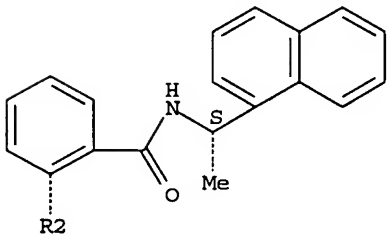

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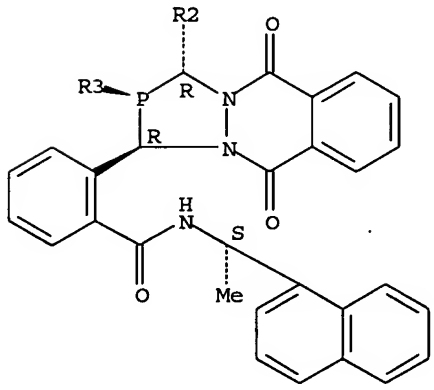

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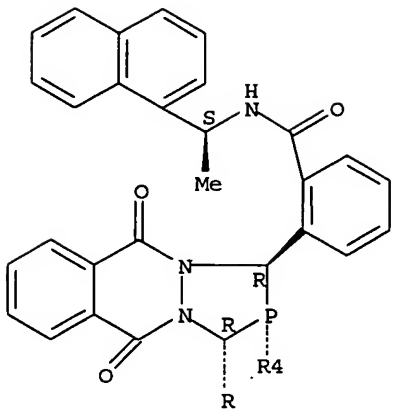

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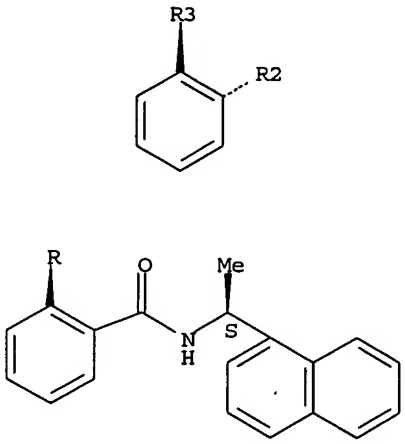
Absolute stereochemistry.

PAGE 1-A



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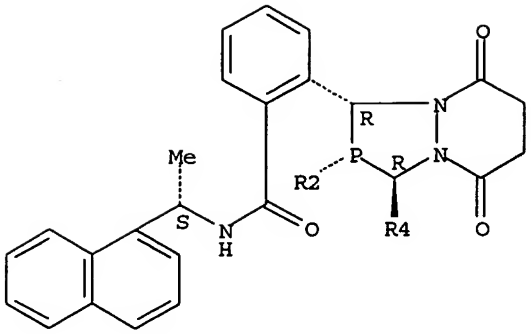

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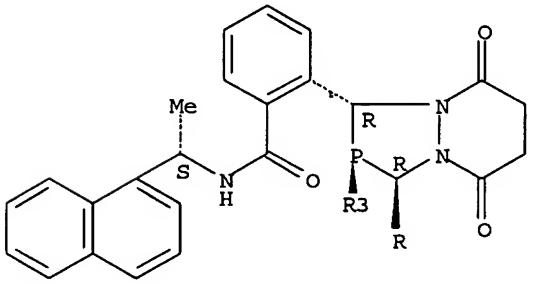

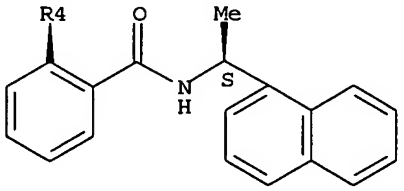

RN 851770-13-3 HCAPLUS
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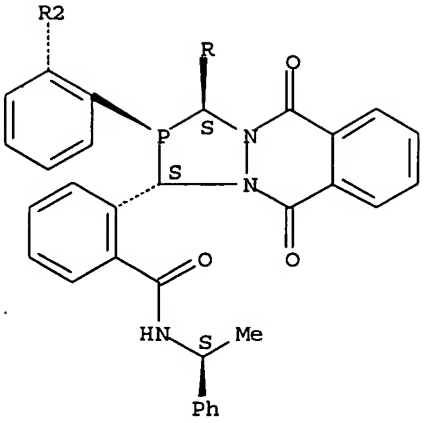
Absolute stereochemistry.

PAGE 1-A



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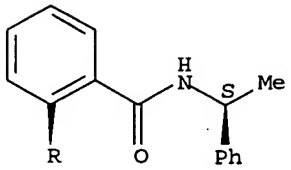

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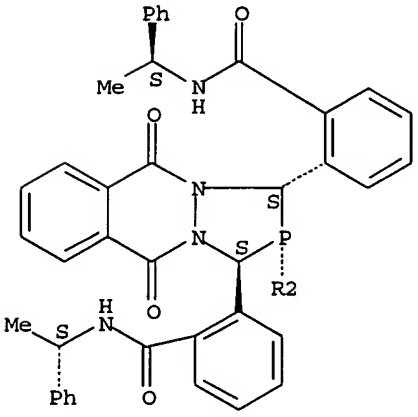

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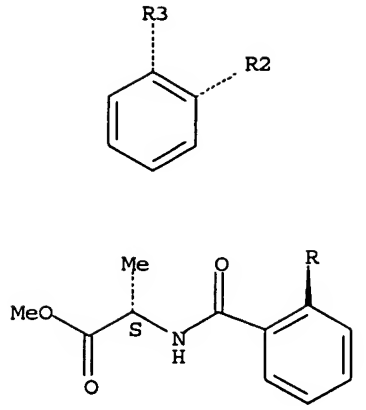
Absolute stereochemistry.

PAGE 1-A



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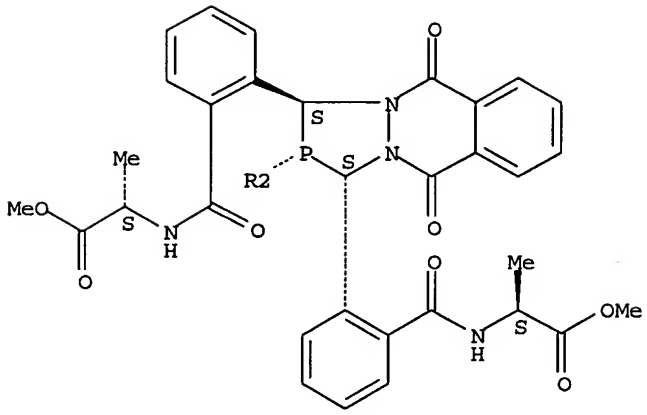

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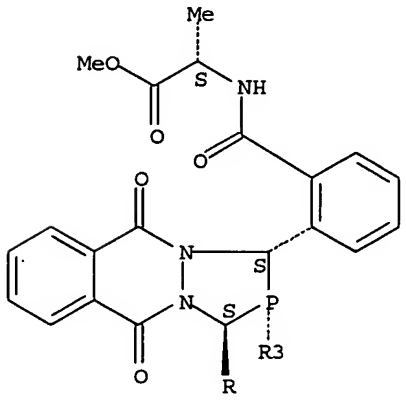

RN 851770-16-6 HCAPLUS

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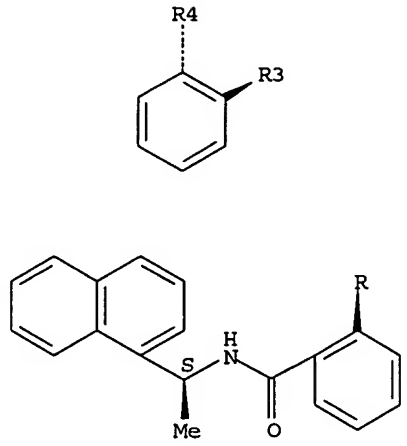
Absolute stereochemistry.

PAGE 1-A



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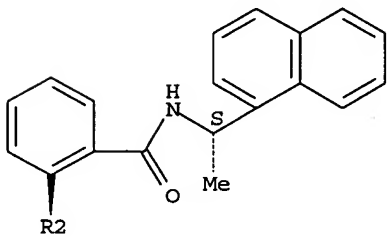

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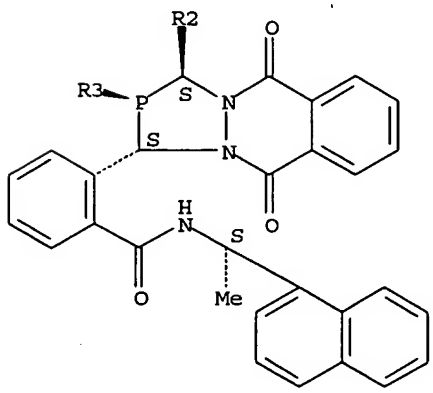

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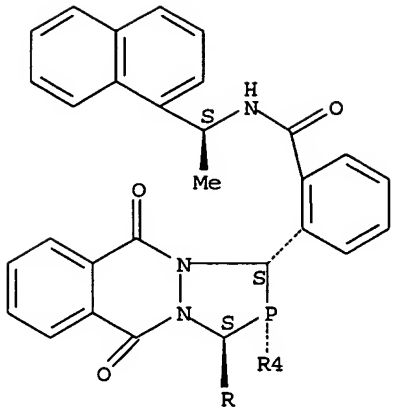

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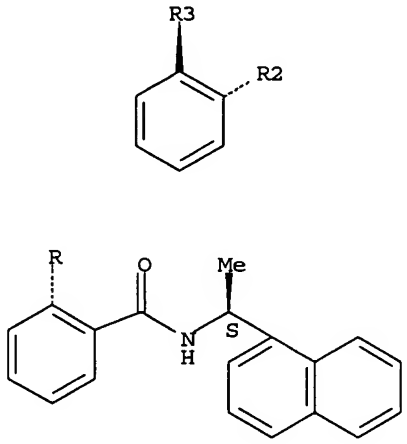
Absolute stereochemistry.

PAGE 1-A



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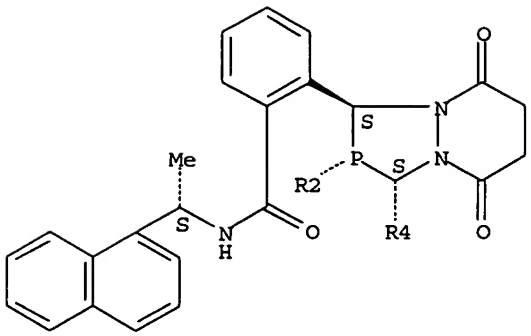

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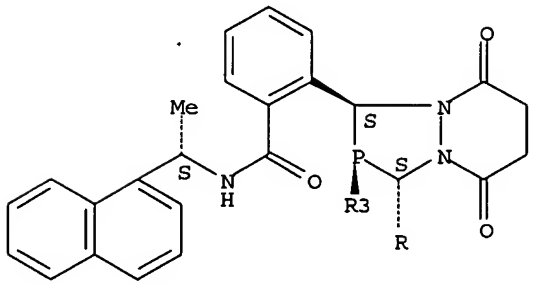
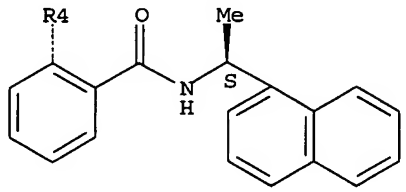




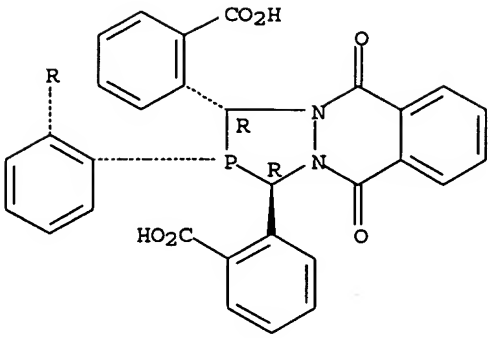
IT 851609-30-8P 851609-31-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and structure of chiral bis(diazaphospholane) ligands for use in rhodium-catalyzed regioselective and stereoselective hydroformylation of alkenes)

RN 851609-30-8 HCAPLUS

CN Benzoic acid, 2,2',2'',2'''-[1,2-phenylenebis[(1R,3R)-5,10-dihydro-5,10-dioxo-1H-[1,2,4]diazaphospholo[1,2-b]phthalazine-2,1,3(3H)-triyl]]tetrakis-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



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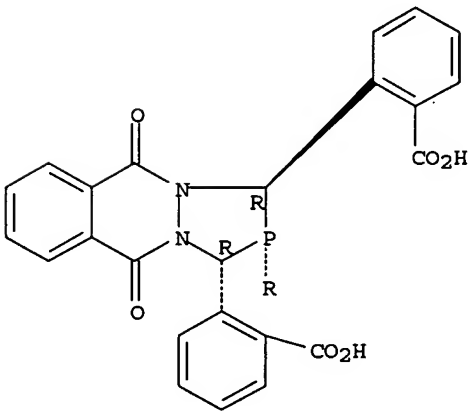

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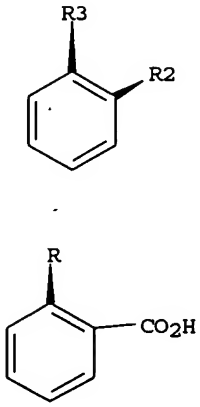
Relative stereochemistry.

PAGE 1-A



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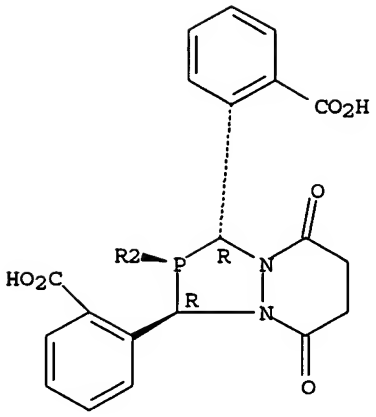

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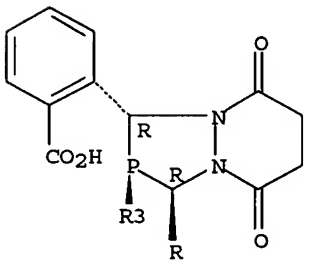

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L39 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:756724 HCAPLUS
DN 141:260889

TI Axially chiral nonracemic phosphites and phosphoramidites having 1,1'-biphenyl-2,2'-diol skeletons and their use in catalytic asymmetric hydrogenation, hydroformylation and addition reactions

IN Ojima, Iwao; Takai, Masaki; Takahashi, Takayoshi

PA Mitsubishi Chemical Corporation, Japan; The Research Foundation of State University of New York

SO PCT Int. Appl., 70 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO2004078766	A1	20040916	2003WO-US05790	20030227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU2003219901	A1	20040928	2003AU-0219901	20030227
WO2004076464	A2	20040910	2004WO-US03367	20040227
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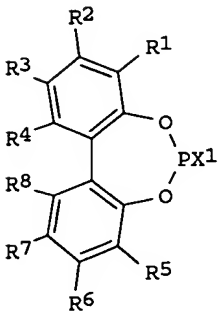
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI 2003WO-US05790 A 20030227

OS MARPAT 141:260889

GI



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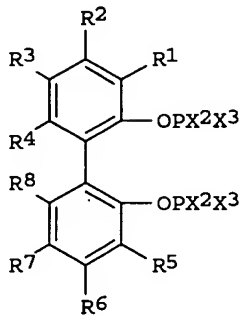


II

AB Novel monodentate configurationally stable axially chiral phosphites and phosphoramidites [(R)- or (S)-I; X1 = OY1, NY2Y3; Y1, Y2, Y3 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, Y2-Y3 may form a ring; R1, R2 = H, (un)substituted secondary or tertiary C3-20 hydrocarbyl; R2, R6 = H, (un)substituted C1-20 alkyl, (un)substituted C1-10 alkoxy, (un)substituted aryl, halogen; R3, R7 = (un)substituted C1-20 hydrocarbyl, (un)substituted C1-10 alkoxy; R4, R8 = C1-4 hydrocarbyl, halogen, C1-4 alkoxy], bidentate phosphites and phosphoramidites [(R)- or (S)-II; X2, X3 = OY4, OY5, resp., or X2X3 =

(NY4Y5)2; Y4, Y5 = (un)substituted alkyl, aryl heteroaryl, Y4-Y5 may form a ring; same R1-R8], preferably I and II with R4 = R8 = Me, are claimed. Also claimed are optically active catalysts comprising mixts. of Group 4-12 metal (or its compound) with ligands I and/or II, preferably Group 8-12 metals, and use of these catalysts in asym. hydrogenation, hydroformylation, allylic substitution, hydrosilylation, and Michael addition reactions, which produce optically active compds. from prochiral precursors. In an example, asym. hydrogenation of di-Me itaconate, catalyzed by composition of 0.1 mol % of [Rh(COD)2]SbF6 (COD = 1,5-cyclooctadiene) and 0.2 mol % of monophosphite (S)-I [X1 = (1S,2R)-2-phenylcyclohexyloxy, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] (preparation given) at 100 psi of H2 at 50° for 20 h affords (R)-di-Me 2-methylsuccinate with 100% conversion and 99.6% ee; the same reaction with use of (S)-I (X1 = OPh, R1 = R2 = R5 = R6 = H, R3 = R4 = R7 = R8 = Me, preparation given) gave (S)-di-Me 2-methylsuccinate with 100% conversion and 96.5% ee. In several further examples, composition of [Rh(COD)(OAc)]2 and (S)-I (X1 = NMe2, R1 = R3 = R5 = R7 = tBu, R4 = R8 = Me, R2 = R6 = H; Rh:ligand = 1:2) catalyzed asym. hydroformylation of styrene (0.1 mol% of Rh), affording, after oxidation, (R)-2-phenylpropanoic acid with 70.1% ee; composition of Cu(II) triflate and (S)-I [Cu:ligand = 1:2, X1 = OPh, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] catalyzed asym. Michael addition of Et2Zn to 2-cyclohexenone affording (S)-3-methylcyclohexanone with 35% ee.

IC ICM C07F-0007/02
ICS C07F-0009/141; C07F-0009/06; C07C-0047/00; C07C-0047/02; C07C-0049/00; C07C-0049/04; C07C-0069/00; C07C-0069/003; C07C-0069/12

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21, 45

IT **Ligands**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(**bidentate**, axially chiral; preparation of axially chiral nonracemic mono- and **diphosphite** and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT **Hydroformylation catalysts**
Hydrogenation catalysts
Hydrosilylation catalysts
Michael reaction catalysts
(stereoselective, axially chiral; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT 80-62-6, Methyl methacrylate **98-83-9**, α-Methylstyrene, reactions 100-42-5, Styrene, reactions
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(asym. hydroformylation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

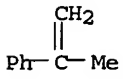
IT **617-52-7**, Dimethyl itaconate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(asym. hydrogenation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT 12097-36-8 **14874-82-9**, (Acetylacetonato)dicarbonylrhodium 130296-28-5
RL: CAT (Catalyst use); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

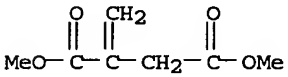
IT **7440-16-6DP**, Rhodium, complex with chiral menthyl binaphthyl phosphite
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation,

Michael addition and allylic alkylation catalysts)

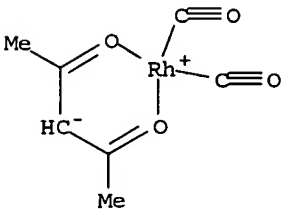
IT **98-83-9**, α-Methylstyrene, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(asym. hydroformylation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
RN 98-83-9 HCAPLUS
CN Benzene, (1-methylethenyl)- (9CI) (CA INDEX NAME)



IT **617-52-7**, Dimethyl itaconate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(asym. hydrogenation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
RN 617-52-7 HCAPLUS
CN Butanedioic acid, methylene-, dimethyl ester (9CI) (CA INDEX NAME)



IT **14874-82-9**, (Acetylacetonato)dicarbonylrhodium
RL: CAT (Catalyst use); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
RN 14874-82-9 HCAPLUS
CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)-
(9CI) (CA INDEX NAME)



IT **7440-16-6DP**, Rhodium, complex with chiral menthyl binaphthyl phosphite
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
RN 7440-16-6 HCAPLUS
CN Rhodium (8CI, 9CI) (CA INDEX NAME)

Rh

RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File

Argyropoulos	1999			US---5952530 A	HCAPLUS
Boyles	2001			WO2001021580	HCAPLUS
Shapiro, R	1997			US---5696280 A	HCAPLUS
Urata	1999			US---5910600 A	HCAPLUS
Wada	2000			JP2000053688	HCAPLUS
Zhang, X	2002			WO2002040491	HCAPLUS

L39 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:740336 HCAPLUS
DN 141:243687
TI Axially chiral nonracemic phosphites and phosphoramidites having 1,1'-biphenyl-2,2'-diol skeletons and their use in catalytic asymmetric hydrogenation, hydroformylation and addition reactions
IN Ojima, Iwao; Takai, Masaki; Takahashi, Takayoshi; Urata, Hisao
PA Mitsubishi Chemical Corporation, Japan; The Research Foundation of State University of New York
SO PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004076464	A2	20040910	2004WO-US03367	20040227
WO2004076464	A3	20041216		
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
WO2004078766	A1	20040916	WO 2003-US305790	20030227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI 2003WO-US05790 A 20030227
OS MARPAT 141:243687
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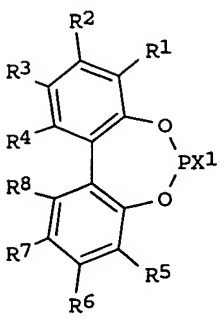

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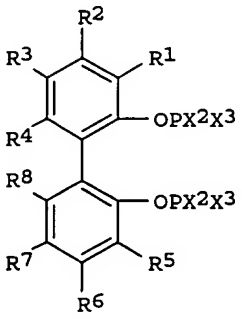


II

AB Novel monodentate configurationally stable axially chiral phosphites and phosphoramidites [(R)- or (S)-I; X1 = OY1, NY2Y3; Y1, Y2, Y3 = (un)substituted alkyl, (un)substituted aryl, (un)substituted heteroaryl, Y2-Y3 may form a ring; R1, R2 = H, (un)substituted secondary or tertiary C3-20 hydrocarbyl; R2, R6 = H, (un)substituted C1-20 alkyl, (un)substituted C1-10 alkoxy, (un)substituted aryl, halogen; R3, R7 = (un)substituted C1-20 hydrocarbyl, (un)substituted C1-10 alkoxy; R4, R8 = C1-4 hydrocarbyl, halogen, C1-4 alkoxy], bidentate phosphites and phosphoramidites [(R)- or (S)-II; X2, X3 = OY4, OY5, resp., or X2X3 = (NY4Y5)2; Y4, Y5 = (un)substituted alkyl, aryl heteroaryl, Y4-Y5 may form a ring; same R1-R8], preferably I and II with R4 = R8 = Me, are claimed. Also claimed are optically active catalysts comprising mixts. of Group 4-12 metal (or its compound) with ligands I and/or II, preferably Group 8-12 metals, and use of these catalysts in asym. hydrogenation, hydroformylation, allylic substitution, hydrosilylation, and Michael addition reactions, which produce optically active compds. from prochiral precursors. In an example, asym. hydrogenation of di-Me itaconate, catalyzed by composition of 0.1 mol % of [Rh(COD)2]SbF6 (COD = 1,5-cyclooctadiene) and 0.2 mol % of monophosphite (S)-I [X1 = (1S,2R)-2-phenylcyclohexyloxy, R1 = R5 = tBu, R3 = R4 = R7 = R8 = Me, R2 = R6 = H] (preparation given) at 100 psi of H2 at 50° for 20 h affords (R)-di-Me 2-methylsuccinate with 100% conversion and 99.6% ee; the same reaction with use of (S)-I (X1 = OPh, R1 = R2 = R5 = R6 = H, R3 = R4 = R7 = R8 = Me, preparation given) gave (S)-di-Me 2-methylsuccinate with 100% conversion and 96.5% ee. In several further examples, composition of [Rh(COD)(OAc)]2 and (S)-I (X1 = NMe2, R1 = R3 = R5 = R7 = tBu, R4 = R8 = Me, R2 = R6 = H; Rh:ligand = 1:2) catalyzed asym. hydroformylation of styrene (0.1 mol% of Rh), affording, after oxidation, (R)-2-phenylpropanoic acid with 70.1% ee; (S)-3-methyl-4-oxobutanenitrile was obtained with 96% regioselectivity and 80% ee by asym hydroformylation of 3-butenenitrile; composition of Cu(II) triflate and (S)-I [Cu:ligand = 1:2, X1 = N[(R)-CHMePh]2, R1 = R3 = R4 = R5 = R7 = R8 = Me, R2 = R6 = H] catalyzed asym. Michael addition of Et2Zn to 2-cycloheptenone affording (S)-3-methylcycloheptanone with 97.5% ee.

IC ICM C07F

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21, 45

IT **Ligands**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(**bidentate**, axially chiral; preparation of axially chiral nonracemic mono- and **diphosphite** and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT **Hydroformylation catalysts**
Hydrogenation catalysts
Hydrosilylation catalysts
Michael reaction catalysts
(stereoselective, axially chiral; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT 557-20-0, Diethylzinc **930-30-3**, 2-Cyclopenten-1-one 930-68-7, 2-Cyclohexen-1-one 1121-66-0, 2-Cyclohepten-1-one
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(asym. Michael addition; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT 80-62-6, Methyl methacrylate **98-83-9**, α-Methylstyrene, reactions 100-42-5, Styrene, reactions 109-75-1, Allyl cyanide
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(asym. hydroformylation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT 80-59-1, Tiglic acid **617-52-7**, Dimethyl itaconate 35356-70-8,

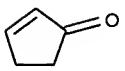
Methyl 2-acetamidoacrylate
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydrogenation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT 12097-36-8 **14874-82-9**, (Acetylacetonato)dicarbonylrhodium
130296-28-5
RL: CAT (Catalyst use); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

IT **7440-16-6DP**, Rhodium, complex with chiral menthyl binaphthyl phosphite
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

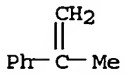
IT **930-30-3**, 2-Cyclopenten-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. Michael addition; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



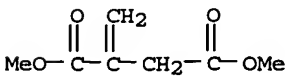
IT **98-83-9**, α-Methylstyrene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydroformylation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 98-83-9 HCAPLUS
CN Benzene, (1-methylethenyl)- (9CI) (CA INDEX NAME)



IT **617-52-7**, Dimethyl itaconate
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. hydrogenation; preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

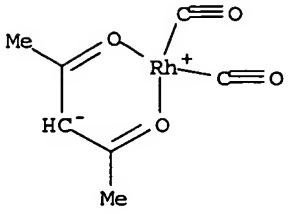
RN 617-52-7 HCAPLUS
CN Butanedioic acid, methylene-, dimethyl ester (9CI) (CA INDEX NAME)



IT **14874-82-9**, (Acetylacetonato)dicarbonylrhodium
RL: CAT (Catalyst use); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)

RN 14874-82-9 HCAPLUS

CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)-
(9CI) (CA INDEX NAME)



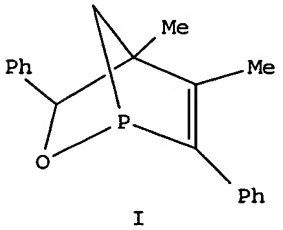
IT 7440-16-6DP, Rhodium, complex with chiral menthyl binaphthyl phosphite
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of axially chiral nonracemic mono- and diphosphite and phosphoramidite ligands for asym. hydrogenation, hydroformylation, Michael addition and allylic alkylation catalysts)
RN 7440-16-6 HCAPLUS
CN Rhodium (8CI, 9CI) (CA INDEX NAME)

Rh

L39 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:307296 HCAPLUS
DN 140:321521
TI Preparation of 1-pnicogena-2-oxanorbornene compounds as cocatalysts for transition metal catalyzed hydroformylation reaction
PA BASF AG, Germany
SO Ger. Offen., 25 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE--10246035	A1	20040415	2002DE-1046035	20021002 <--
PRAI 2002DE-1046035		20021002 <--		

OS CASREACT 140:321521; MARPAT 140:321521
GI



I

AB The present invention concerns the preparation of compds., which contains at least one 1-pnicogena-2-oxabicyclo[2.2.1]heptene structural element, useful as cocatalysts, for transition metal catalyzed hydroformylation reaction. Thus, hetero-Diels-Alder reaction of 3,4-dimethyl-1-

phenylphosphole with benzaldehyde in xylene at 150° for 2 h gave title compound I. The Rh(CO)2(acac)/I catalyzed-hydroformylation of 1-octene is also described.

IC ICM C07F-0009/655
ICS C07F-0009/80; C07F-0009/90; B01J-0031/22; C07C-0045/50

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 67

IT **Hydroformylation catalysts**
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

IT **Alkenes, reactions**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

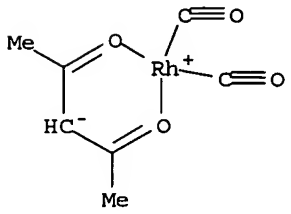
IT **14874-82-9**, (Acetylacetonato)dicarbonylrhodium
RL: CAT (Catalyst use); USES (Uses)
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

IT 100-52-7, Benzaldehyde, reactions **111-66-0**, 1-Octene 123-11-5, 4-Methoxybenzaldehyde, reactions 459-57-4, 4-Fluorobenzaldehyde 623-27-8, 1,4-Benzenedicarboxaldehyde 1162-70-5, 1,2,5-Triphenylphosphole 13381-22-1, 2,2'-Dilithiodiphenyl ether 30540-36-4, 3,4-Dimethyl-1-phenylphosphole 63762-32-3, 2,5-Dilithiofuran 115076-24-9, 1-Cyano-3,4-Dimethylphosphole 187885-04-7, 3,4-Dimethyl-1-(2-pyridyl)phosphole 210532-76-6, 1-(2-Bromophenyl)-3,4-dimethylphosphole 678188-51-7
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

IT 678188-46-0P 678188-47-1P **678188-48-2P** 678188-49-3P 678188-50-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

IT **14874-82-9**, (Acetylacetonato)dicarbonylrhodium
RL: CAT (Catalyst use); USES (Uses)
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

RN 14874-82-9 HCAPLUS
CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)-(9CI) (CA INDEX NAME)



IT **111-66-0**, 1-Octene
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

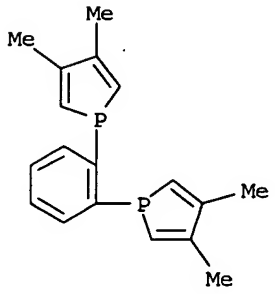
RN 111-66-0 HCAPLUS
CN 1-Octene (8CI, 9CI) (CA INDEX NAME)

$H_2C{=}CH{-}(CH_2)_5{-}Me$

IT **678188-48-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pnicogenaoxanorbornene compds. as cocatalysts for transition metal catalyzed alkene hydroformylation)

RN 678188-48-2 HCAPLUS
CN 1H-Phosphole, 1,1'-(1,2-phenylene)bis[3,4-dimethyl- (9CI) (CA INDEX NAME)



L39 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:818434 HCAPLUS
DN 139:307895
TI Preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asymmetric reactions
IN Boerner, Armin; Holz, Jens; Monsees, Axel; Riermeier, Thomas; Kadyrov, Renat; Schneider, Carsten A.; Dingerdissen, Uwe; Drauz, Karlheinz
PA Degussa A.-G., Germany
SO PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO2003084971	A1	20031016	2003WO-EP02162	20030303	<--
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	EP---1490379	A1	20041229	2003EP-0708169	20030303	<--
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	JP2005529868	T2	20051006	2003JP-0582168	20030303	<--
	US2005209455	A1	20050922	2005US-0508537	20050512	<--
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OS CASREACT 139:307895; MARPAT 139:307895
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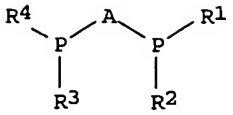


I

AB The present invention relates to the preparation of ligands, I (R1-R4 = independent of each other C1-8 alkyl, C2-8 alkoxyalkyl, C6-18 aryl, C7-19 aralkyl, C3-18 heteroaryl, C4-19 heteroaralkyl, C1-8-alkyl-C6-18-aryl, C1-8-alkyl-C3-18-heteroaryl, C3-8-cycloalkyl, C1-8-alkyl-C3-8-cycloalkyl, C3-8-cycloalkyl-C1-8-alkyl; R1-R2, and/or R3-R4 = C3-5 alkylene bridge mono or polysubstituted with C1-8 alkyl, HO-(C1-8)-alkyl, (C1-8)-alkoxy, (C2-8)-alkoxyalkyl, (C6-18)-aryl, etc.; A = (un)substituted heterocyclic structure), useful as cocatalysts with transition metal catalyzed asym. reactions, is described. Thus, reaction of 2,3-dichloromaleic anhydride with (R,R)-2,5-dimethyl-1-trimethylsilylphospholane (preparation given) gave 2,3-bis[(R,R)-2,5-dimethyl-phospholanyl]maleic anhydride which on treatment with [Rh(COD)2]BF4 in THF gave the catalyst which was used for asym. hydrogenation of unsatd. substrates, e.g. Me acetamidocinnamate.

IC ICM C07F-0009/50
ICS C07F-0009/6568; C07F-0009/655; C07F-0009/6509; C07F-0009/6506; C07F-0015/00; B01J-0031/24; C07B-0053/00; C07C-0045/00; C07C-0231/18; C07M-0007/00

CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23

IT Aldol condensation catalysts
Hydroformylation catalysts
Hydrogenation catalysts
Hydrosilylation catalysts
Rearrangement catalysts
(stereoselective; preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)

IT **7439-88-5D**, Iridium, bisphosphine complexes **7440-02-0D**, Nickel, bisphosphine complexes **7440-04-2D**, Osmium, bisphosphine complexes **7440-05-3D**, Palladium, bisphosphine complexes **7440-06-4D**, Platinum, bisphosphine complexes **7440-16-6D**, Rhodium, bisphosphine complexes **7440-18-8D**, Ruthenium, bisphosphine complexes **7440-48-4D**, Cobalt, bisphosphine complexes 7440-50-8D, Copper, bisphosphine complexes 210057-23-1
RL: CAT (Catalyst use); USES (Uses)
(preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)

IT 617-52-7, Dimethyl itaconate 638-21-1, Phenylphosphine 1122-17-4 15573-38-3, Tris(trimethylsilyl)phosphine 33912-78-6 35138-22-8, Bis(1,5-cyclooctadiene)rhodium(1+) tetrafluoroborate 59624-91-8, Lithium bis(trimethylsilyl)phosphide 72569-96-1 88010-06-4 220224-82-8 245727-69-9 464926-43-0
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)

IT 129647-10-5P 505092-85-3P **505092-86-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)

IT **7439-88-5D**, Iridium, bisphosphine complexes **7440-02-0D**, Nickel, bisphosphine complexes **7440-04-2D**, Osmium, bisphosphine complexes **7440-05-3D**, Palladium, bisphosphine complexes **7440-06-4D**, Platinum, bisphosphine complexes **7440-16-6D**, Rhodium, bisphosphine complexes **7440-18-8D**, Ruthenium, bisphosphine complexes **7440-48-4D**, Cobalt, bisphosphine complexes

RL: CAT (Catalyst use); USES (Uses)
(preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)
RN 7439-88-5 HCAPLUS
CN Iridium (8CI, 9CI) (CA INDEX NAME)

Ir

RN 7440-02-0 HCAPLUS
CN Nickel (8CI, 9CI) (CA INDEX NAME)

Ni

RN 7440-04-2 HCAPLUS
CN Osmium (8CI, 9CI) (CA INDEX NAME)

Os

RN 7440-05-3 HCAPLUS
CN Palladium (8CI, 9CI) (CA INDEX NAME)

Pd

RN 7440-06-4 HCAPLUS
CN Platinum (8CI, 9CI) (CA INDEX NAME)

Pt

RN 7440-16-6 HCAPLUS
CN Rhodium (8CI, 9CI) (CA INDEX NAME)

Rh

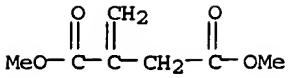
RN 7440-18-8 HCAPLUS
CN Ruthenium (8CI, 9CI) (CA INDEX NAME)

Ru

RN 7440-48-4 HCAPLUS
CN Cobalt (8CI, 9CI) (CA INDEX NAME)

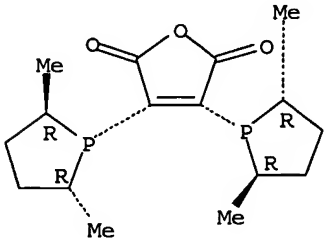
Co

IT 617-52-7, Dimethyl itaconate
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)
RN 617-52-7 HCAPLUS
CN Butanedioic acid, methylene-, dimethyl ester (9CI) (CA INDEX NAME)



IT 505092-86-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asym. reactions)
RN 505092-86-4 HCAPLUS
CN 2,5-Furandione, 3,4-bis[(2R,5R)-2,5-dimethyl-1-phospholanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Holz, J	2003	68	1701	JOURNAL OF ORGANIC C	HCAPLUS
Solvias Ag	2003			WO--03031456 A	HCAPLUS

L39 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2003:155116 HCAPLUS
DN 138:205227
TI Asymmetric catalysis based on chiral phospholanes
IN Zhang, Xumu
PA The Penn State Research Foundation, USA
SO U.S. Pat. Appl. Publ., 41 pp., Cont.-in-part of U. S. 6,337,406.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US2003040629	A1	20030227	2001US-0992551	20011106 <--
	US---6727377	B2	20040427		
	US---6337406	B1	20020108	1999US-0377065	19990819 <--
	WO2003040149	A2	20030515	2002WO-US35484	20021106 <--
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US2004176618	A1	20040909	2004US-0791320	20040302 <--
	US---6946569	B2	20050920		

PRAI 1998US-097473P P 19980821 <--
1999US-0377065 A2 19990819 <--
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2001US-0992551 A 20011106 <--
OS MARPAT 138:205227
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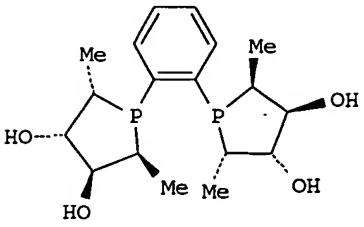


I

AB Chiral phosphine ligands derived from chiral natural products, including D-mannitol and tartaric acid, were prepared The ligands, e.g. (I) (preparation given), contain one or more 5-membered phospholane rings with multiple chiral centers, and provide high stereoselectivity in asym. reactions. For example, [Rh(COD)2]PF6-catalyzed asym. hydrogenation of dehydroamino acid derivs. in the presence of I gave products in up to 99% enantiomeric excess.

IC ICM C07F-0009/653
ICS C07F-0009/547

INCL 548112000; 556404000; 568012000

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21, 33

IT **Alkenes, reactions**
Imines
Ketones, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(asym. hydrogenation of; preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

IT Aldol condensation catalysts
Cyclopropanation catalysts
Diels-Alder reaction catalysts
Hydride transfer catalysts
Hydroboration catalysts
Hydroformylation catalysts
Hydrogenation
Hydrogenation catalysts
Hydrosilylation catalysts
Michael reaction catalysts
(stereoselective; preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

IT **97-65-4**, reactions **617-52-7** 5429-56-1 5469-45-4
25957-50-0 35356-70-8 39239-88-8 52386-78-4 68280-85-3
68762-59-4 74839-85-3 92635-04-6 92635-05-7 111649-72-0
132165-60-7 132165-61-8 162555-59-1 171095-23-1 224186-20-3
224186-21-4 259752-09-5 259752-11-9 259752-12-0 259752-13-1
497859-91-3
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(asym. hydrogenation reaction; preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

IT **3375-31-3**, Palladium (II) acetate 12012-95-2 **12092-47-6**
12112-67-3 **14874-82-9**, Dicarbonylacetylacetonato rhodium
(I) 35138-22-8 50982-12-2 **51364-51-3** 59420-05-2
62793-31-1 99326-34-8 130296-28-5 162412-87-5 436863-50-2

499984-41-7 499984-42-8
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

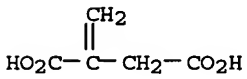
IT **248244-33-9P** 259752-00-6P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

IT **215930-44-2P 248244-34-0P 259752-01-7P**
259752-06-2P 259752-07-3P 259752-16-4P 259752-17-5P 259752-18-6P
259752-19-7P 259752-20-0P 259752-22-2P 259752-24-4P
259752-26-6P 488760-58-3P 499984-38-2P 499984-39-3P
499984-53-1P 499984-56-4P 499984-71-3P **500000-10-2P**
500000-11-3P 500000-12-4P **500000-13-5P 500000-14-6P**
500000-15-7P 500000-16-8P 500000-17-9P **500000-18-0P**
500000-19-1P 500000-20-4P 500102-04-5P 500102-05-6P
500117-78-2P 500117-79-3P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

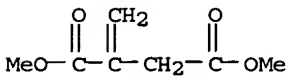
IT 3969-59-3P 3969-84-4P 53754-41-9P 63700-05-0P 74044-75-0P
159716-51-5P 221022-89-5P 259535-67-6P 259752-03-9P
259752-04-0P 259752-08-4P 495385-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

IT **97-65-4**, reactions **617-52-7**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(asym. hydrogenation reaction; preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

RN 97-65-4 HCAPLUS
CN Butanedioic acid, methylene- (9CI) (CA INDEX NAME)

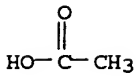


RN 617-52-7 HCAPLUS
CN Butanedioic acid, methylene-, dimethyl ester (9CI) (CA INDEX NAME)



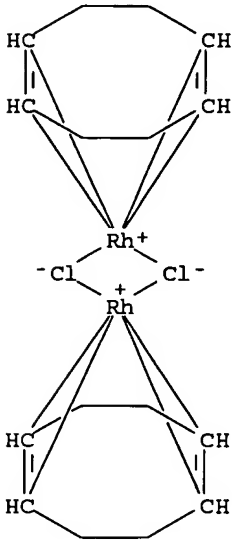
IT 3375-31-3, Palladium (II) acetate **12092-47-6**
12112-67-3 14874-82-9, Dicarbonylacetylacetonato rhodium (I) **51364-51-3**
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

RN 3375-31-3 HCAPLUS
CN Acetic acid, palladium(2+) salt (8CI, 9CI) (CA INDEX NAME)

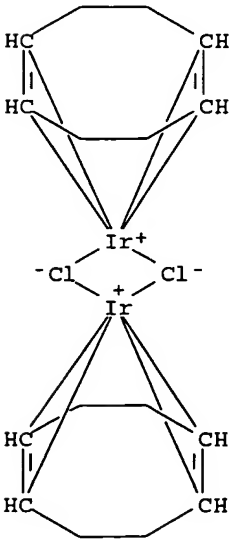


●1/2 Pd(II)

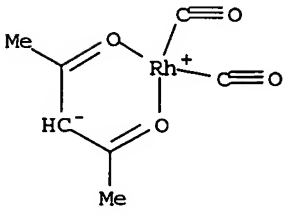
RN 12092-47-6 HCAPLUS
CN Rhodium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



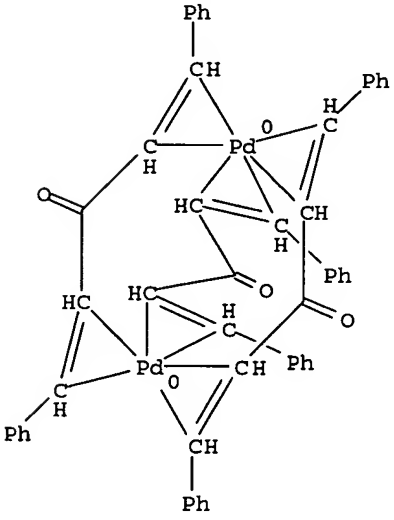
RN 12112-67-3 HCAPLUS
CN Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



RN 14874-82-9 HCAPLUS
CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)-
(9CI) (CA INDEX NAME)

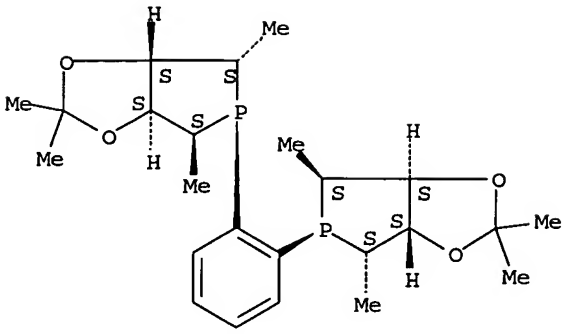


RN 51364-51-3 HCAPLUS
CN Palladium, tris[μ-[(1,2-η:4,5-η)-(1E,4E)-1,5-diphenyl-1,4-
pentadien-3-one]]di- (9CI) (CA INDEX NAME)



IT 248244-33-9P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)
RN 248244-33-9 HCAPLUS
CN 5H-Phospholo[3,4-d]-1,3-dioxole, 5,5'-(1,2-phenylene)bis[tetrahydro-2,2,4,6-tetramethyl-, (3aS,3'aS,4S,4'S,6S,6'S,6aS,6'aS)- (9CI) (CA INDEX NAME)

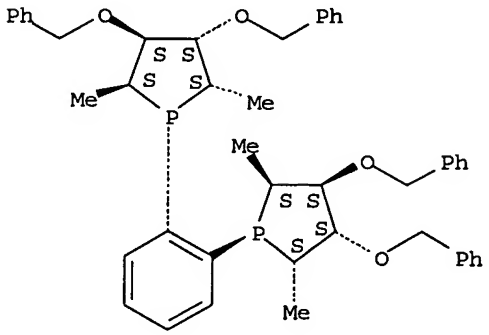
Absolute stereochemistry. Rotation (+).



IT **215930-44-2P 248244-34-0P 259752-01-7P**
259752-26-6P 500000-10-2P 500000-13-5P
500000-14-6P 500000-18-0P 500000-19-1P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)

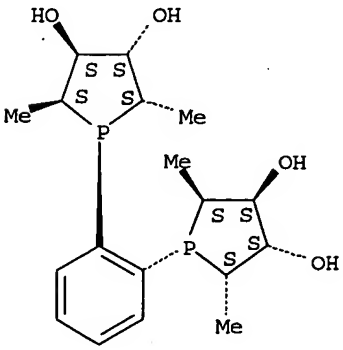
RN 215930-44-2 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-dimethyl-3,4-bis(phenylmethoxy)-, (2S,2'S,3S,3'S,4S,4'S,5S,5'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



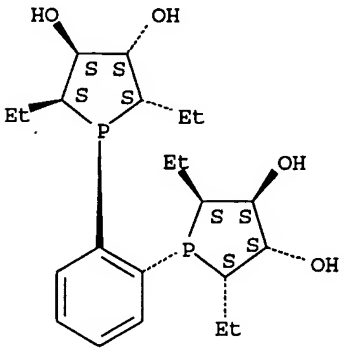
RN 248244-34-0 HCAPLUS
CN 3,4-Phospholanediol, 1,1'-(1,2-phenylene)bis[2,5-dimethyl-, (2S,2'S,3S,3'S,4S,4'S,5S,5'S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 259752-01-7 HCAPLUS
CN 3,4-Phospholanediol, 1,1'-(1,2-phenylene)bis[2,5-diethyl-, (2S,2'S,3S,3'S,4S,4'S,5S,5'S)- (9CI) (CA INDEX NAME)

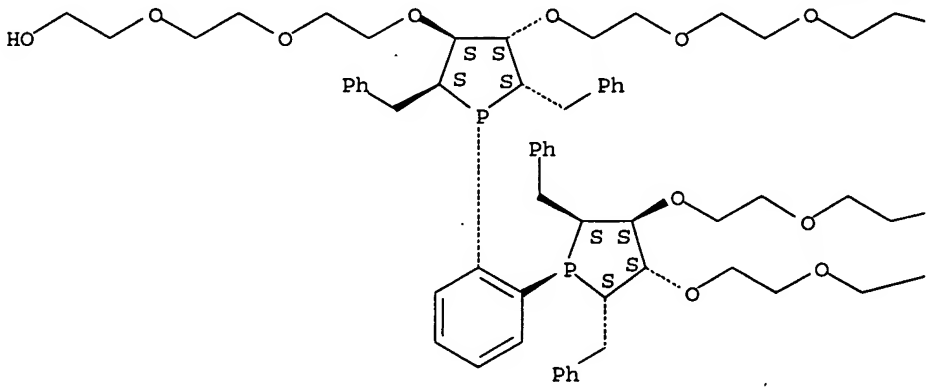
Absolute stereochemistry. Rotation (+).



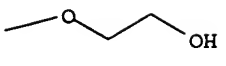
RN 259752-26-6 HCAPLUS
CN Ethanol, 2,2',2'',2''-[1,2-phenylenebis[[(2S,3S,4S,5S)-2,5-bis(phenylmethyl)-1,3,4-phospholanetriyl]bis(oxy-2,1-ethanediyloxy-2,1-ethanediyloxy)]]tetrakis- (9CI) (CA INDEX NAME)

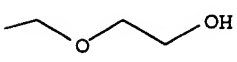
Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



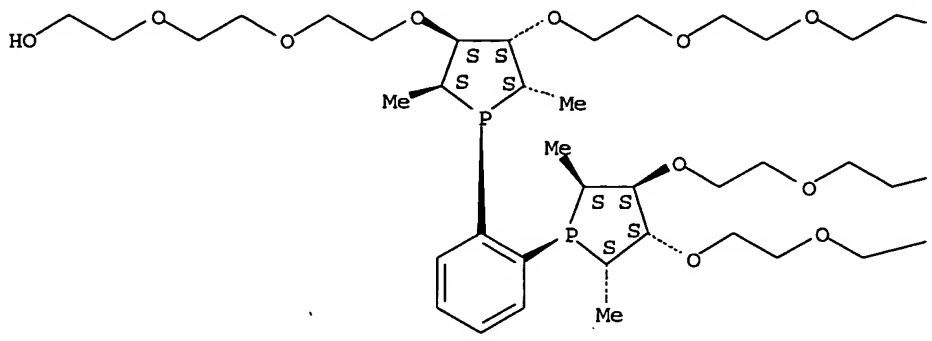


RN 500000-10-2 HCAPLUS

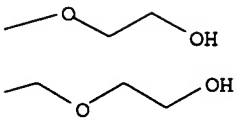
CN Ethanol, 2,2',2'',2'''-[1,2-phenylenebis[[(2S,3S,4S,5S)-2,5-dimethyl-1,3,4-phospholanetriyl]bis(oxy-2,1-ethanediyloxy-2,1-ethanediyloxy)]]tetrakis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

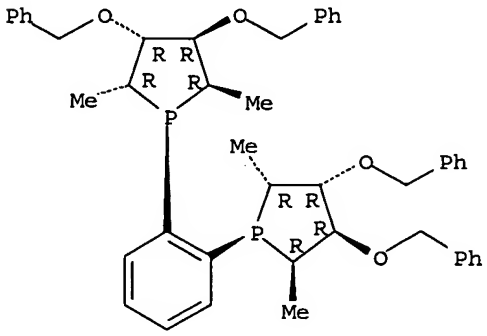


PAGE 1-B



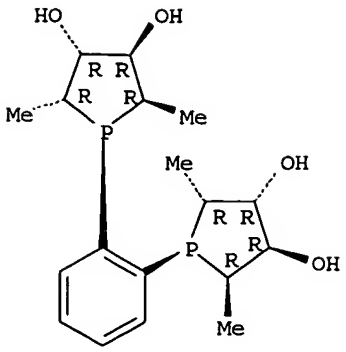
RN 500000-13-5 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-dimethyl-3,4-bis(phenylmethoxy)-, (2R,2'R,3R,3'R,4R,4'R,5R,5'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 500000-14-6 HCAPLUS
CN 3,4-Phospholanediol, 1,1'-(1,2-phenylene)bis[2,5-dimethyl-, (2R,2'R,3R,3'R,4R,4'R,5R,5'R)- (9CI) (CA INDEX NAME)

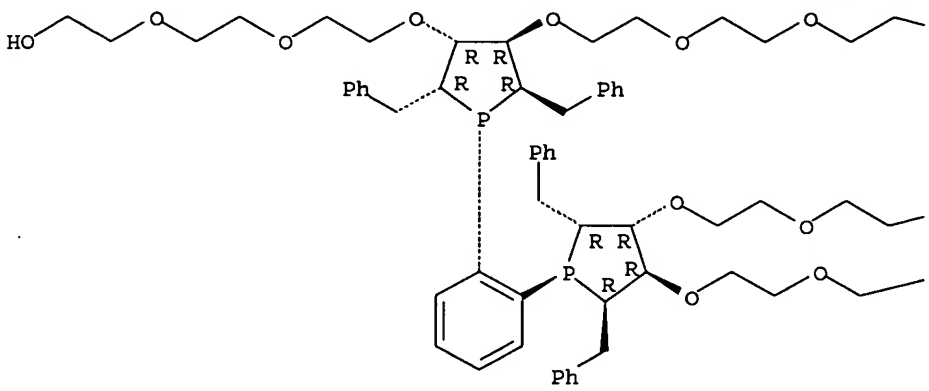
Absolute stereochemistry.



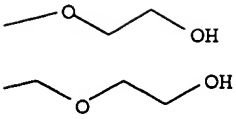
RN 500000-18-0 HCAPLUS
CN Ethanol, 2,2',2'',2'''-[1,2-phenylenebis[[(2R,3R,4R,5R)-2,5-bis(phenylmethyl)-1,3,4-phospholanetriyl]bis(oxy-2,1-ethanediyloxy-2,1-ethanediyloxy)]]tetrakis- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

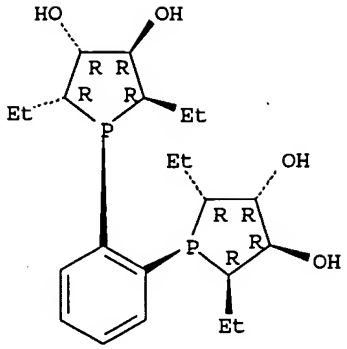


PAGE 1-B



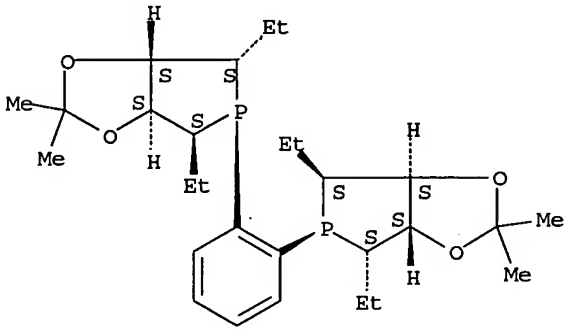
RN 500000-19-1 HCAPLUS
CN 3,4-Phospholanediol, 1,1'-(1,2-phenylene)bis[2,5-diethyl-, (2R,2'R,3R,3'R,4R,4'R,5R,5'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 259752-04-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of chiral phospholanes as cocatalysts with transition metals for asym. catalysis of organic reactions)
RN 259752-04-0 HCAPLUS
CN 5H-Phospholo[3,4-d]-1,3-dioxole, 5,5'-(1,2-phenylene)bis[4,6-diethyltetrahydro-2,2-dimethyl-, (3aS,3'aS,4S,4'S,6S,6'S,6aS,6'aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L39 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2001:855302 HCAPLUS
DN 136:247673
TI Synthesis and characterization of {[(COD)Rh(bis-(2R,3R)-2,5-diethylphospholanobenzene)]+BARF-} for use in homogeneous catalysis in supercritical carbon dioxide
AU Guzel, Bilgehan; Omary, Mohammad A.; Fackler, John P.; Akgerman, Aydin
CS Laboratory for Molecular Structure and Bonding, Department of Chemistry, Texas A&M University, College Station, TX, 77843-3012, USA
SO Inorganica Chimica Acta (2001), 325(1,2), 45-50
CODEN: ICHAA3; ISSN: 0020-1693
PB Elsevier Science S.A.
DT Journal
LA English
OS CASREACT 136:247673
AB Reaction of [(COD)2Cl2Rh] (COD: cyclo-octadiene) with sodium tetrakis((3,5-trifluoromethyl)phenyl)borate (NaBARF) in the presence of an excess of COD yields [(COD)2Rh]+BARF-. The COD ligands are readily displaced by the bidentate ligand 1,2-bis((2R,5R)-2,5-diethylphosphalono)benzene (Et-DuPHOS) to form [(COD)Rh(Et-DuPHOS)]BARF, the structure of which was determined by x-ray crystallog. BARF was selected

as the counterion in order to achieve solubility in supercrit. carbon dioxide for use in asym. hydrogenation and hydroformylation reactions. D.-functional theory calcns. were used to study the intermediates in asym. hydroformylation of styrene. The energies of the two-enantiomer models differ by 11.3 kcal mol-1.

CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 75

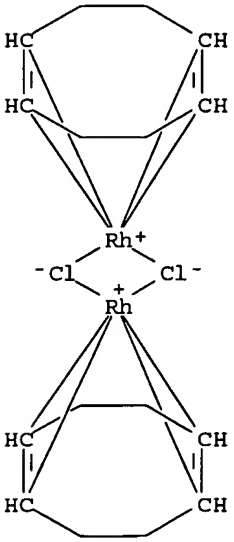
IT **Hydroformylation catalysts**
(stereoselective; preparation of rhodium diethylphospholanobenzene cyclooctadiene trifluoromethylphenylborate for use in homogeneous catalysis in supercrit. carbon dioxide)

IT **111-78-4**, Cycloocta-1,5-diene **12092-47-6**
393801-74-6
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation and characterization of rhodium diethylphospholanobenzene cyclooctadiene trifluoromethylphenylborate for use in homogeneous catalysis in supercrit. carbon dioxide)

IT **111-78-4**, Cycloocta-1,5-diene **12092-47-6**
393801-74-6
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(preparation and characterization of rhodium diethylphospholanobenzene cyclooctadiene trifluoromethylphenylborate for use in homogeneous catalysis in supercrit. carbon dioxide)

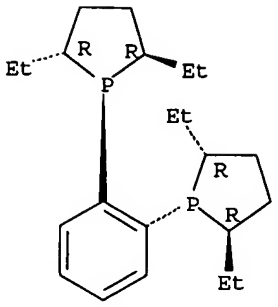
RN 111-78-4 HCAPLUS
CN 1,5-Cyclooctadiene (6CI, 8CI, 9CI) (CA INDEX NAME)

RN 12092-47-6 HCAPLUS
CN Rhodium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (9CI) (CA INDEX NAME)



RN 393801-74-6 HCAPLUS
CN Phospholane, 1,1'-(1,2-phenylene)bis[2,5-diethyl-, (2R,2'R,5R,5'R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RETABLE

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Berge, S	1991		416	NMR Spectroscopy of	
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Frisch, M	1998			Gaussian 98 (Revisio	
Green, M	1971		2334	J Chem Soc A	HCAPLUS
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Ikariya, T	2000	4	39	Catal Surv Jpn	HCAPLUS
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Miehlich, B	1989	157	200	Chem Phys Lett	HCAPLUS
Molecular Simulations I	1999			Cerius2, Release 4.0	
Morgenstern, D	1996	626	132	ACS Symp Ser	HCAPLUS
Nishida, H	1984	57	2600	Bull Chem Soc Jpn	HCAPLUS
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Nozaki, K	2000	19	2031	Organometallics	HCAPLUS
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Parr, R	1989			Density-Functional T	
Sakai, N	1993	115	7033	J Am Chem Soc	HCAPLUS
Sakai, N	1994		395	J Chem Soc, Chem Com	HCAPLUS
Schrock, R	1971	93	2397	J Am Chem Soc	

L39 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:608754 HCAPLUS
DN 133:193276
TI Chiral diazaphospholidine ligands
IN Wills, Martin; Breeden, Simon
PA University of Warwick, UK
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2

Ans 12 of 12

DT Patent
LA English
FAN.CNT 1

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PI	WO2000050430	A1	20000831	2000WO-GB00538	20000216 <--
	W: JP, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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	EP---1155024	B1	20030709		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
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	US---6717011	B1	20040406	2001US-0914144	20011212 <--
PRAI	1999GB-0003973	A	19990223 <--		
	2000GB-0000428	A	20000111 <--		
	2000WO-GB00538	W	20000216 <--		

OS CASREACT 133:193276; MARPAT 133:193276
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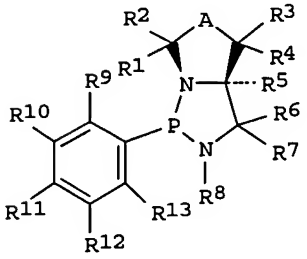

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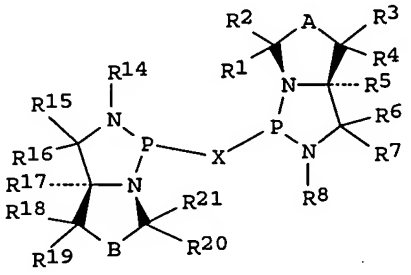

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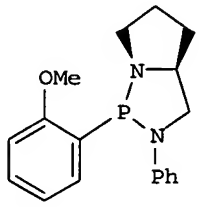


III

AB The application relates to diazaphospholidine compds. I and II (A, B = independently selected from C(R22R23) and C(R22R23)C(R24R25); R1, R2, R3, R4, R18, R19, R20, R21, R22, R23, R24, R25 = may or may not be present and each may be independently selected from H, halo, OH, organosulfonyl, SH, NO2, NH2, :O, :S, straight chain, branched chain, cyclic, saturated, non-saturated, substituted or non-substituted alkyl, hydroalkyl, carboalkyl, alkoxy, amino, alkenyl, aryl and CH2Ar (Ar = aryl or substituted aryl), C1-6, Si1-6 silane; R1, R2, R3, R4, R18, R19, R20, R21, R22, R23, R24 and/or R25 group is not present an unsatd. bond is formed; R5, R17 = H, NH2, OH, halo, (un)substituted straight or branched chain alkyl or aryl; R6, R7, R15, R16 = independently selected from halo, OH, SO2, SH, NO2, NH2, straight chain, branched chain, cyclic, saturated, non-saturated, (un)substituted alkyl, carboalkyl, alkoxy, alkenyl, aryl, Si1-6 silane; R8, R14 = H, straight, branched, cyclic, saturated, non-saturated, (un)substituted

alkyl, carboalkyl, alkoxy, alkenyl, aryl, CH2Ar; R9, R10, R11, R12, R13 = independently selected from halide OH, SO2, SH, NO2, NH2, straight chain, branched chain, cyclic, saturated, non-saturated, (un)substituted alkyl, carboalkyl, alkoxy, amino, alkenyl, aryl, CH2Ar, or a silane containing 1 to 6 silicon atoms; and X = linking group containing 1 to 12 atoms; or a salt thereof). These compds. may be used as catalysts for asym. catalyst of organic reactions. Thus, reaction of (S)-2-(phenylaminomethyl)pyrrolidine with 2-anisyl-bis(dimethylamino)phosphine in PhMe gave title ligand III, which was used as catalyst with tris(dibenzylideneacetone)dipalladium complex for allylic substitution reaction of 1,3-diphenyl-3-acetoxy-1-propene with di-Me malonate.

IC ICM C07F-0009/6584

CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 21, 35

IT **Hydroformylation catalysts**
(asym.; preparation of chiral diazaphospholidine ligand as cocatalyst for rhodium catalyzed asym. hydroformylation reaction)

IT **Alkenes, reactions**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of chiral diazaphospholidine ligand as cocatalyst for palladium catalyzed alkene hydrosilylation reaction)

IT **289622-37-3P 289622-38-4P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as asym. cocatalyst for organic reactions)

IT **51364-51-3**, Tris(dibenzylideneacetone)dipalladium
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral diazaphospholidine ligand as cocatalyst for palladium catalyzed allylic substitution reaction)

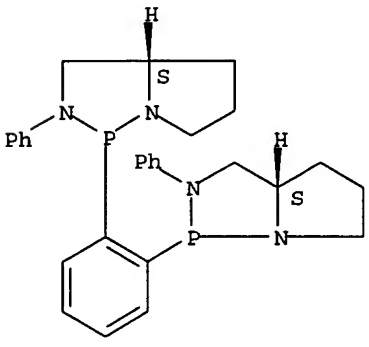
IT **14874-82-9**
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral diazaphospholidine ligand as cocatalyst for rhodium catalyzed asym. hydroformylation reaction)

IT **289622-38-4P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as asym. cocatalyst for organic reactions)

RN 289622-38-4 HCAPLUS

CN 1H-Pyrrolo[1,2-c][1,3,2]diazaphosphole, 1,1'-(1,2-phenylene)bis[hexahydro-2-phenyl-, (3aS,3'aS)- (9CI) (CA INDEX NAME)

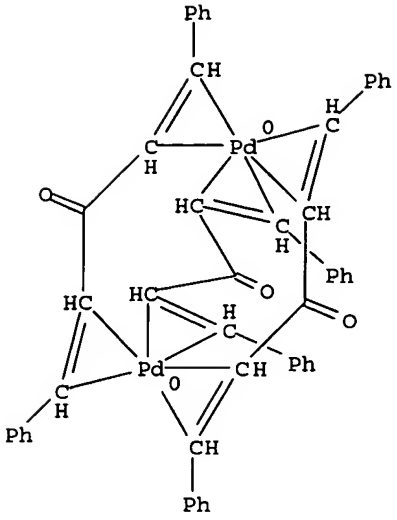
Absolute stereochemistry.



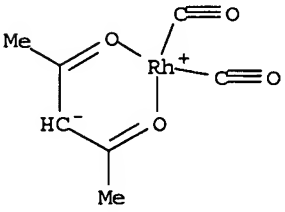
IT **51364-51-3**, Tris(dibenzylideneacetone)dipalladium
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral diazaphospholidine ligand as cocatalyst for palladium catalyzed allylic substitution reaction)

RN 51364-51-3 HCAPLUS

CN Palladium, tris[μ-[(1,2-η:4,5-η)-(1E,4E)-1,5-diphenyl-1,4-pentadien-3-one]]di- (9CI) (CA INDEX NAME)



IT 14874-82-9
RL: CAT (Catalyst use); USES (Uses)
(preparation of chiral diazaphospholidine ligand as cocatalyst for rhodium catalyzed asym. hydroformylation reaction)
RN 14874-82-9 HCAPLUS
CN Rhodium, dicarbonyl(2,4-pentanedionato-κO,κO')-, (SP-4-2)-
(9CI) (CA INDEX NAME)



RETABLE

Referenced Author (RAU)	Year (RPY)	VOL (RVL)	PG (RPG)	Referenced Work (RWK)	Referenced File
Brunel, J	1997	529	285	JOURNAL OF ORGANOMET	
Brunel, J	1998	39	2961	TETRAHEDRON LETTERS	HCAPLUS
Muchow, G	1998	54	10435	TETRAHEDRON	HCAPLUS

=> => b casre
FILE 'CASREACT' ENTERED AT 16:16:10 ON 10 AUG 2006
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FILE CONTENT:1840 - 6 Aug 2006 VOL 145 ISS 6

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*                                                          *
*     CASREACT now has more than 10 million reactions      *
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> d que sta l40
L40             STR

RRT                 RRT          RRT

P---C~C---P         C===C        M 7
1   2   3   4       5   6

NODE ATTRIBUTES:
NSPEC   IS R      AT   1
NSPEC   IS R      AT   4
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   7

STEREO ATTRIBUTES: NONE


=> d bib abs crd 142 tot

L42  ANSWER 1 OF 1  CASREACT  COPYRIGHT 2006 ACS on STN
AN   143:60067  CASREACT
TI   Chiral Palladium(0) trans-Stilbene Complexes: Synthesis, Structure, and
     Oxidative Addition of Phenyl Iodide
AU   Brunker, Tim J.; Blank, Natalia F.; Moncarz, Jillian R.; Scriban, Corina;
     Anderson, Brian J.; Glueck, David S.; Zakharov, Lev N.; Golen, James A.;
     Sommer, Roger D.; Incarvito, Christopher D.; Rheingold, Arnold L.
CS   6128 Burke Laboratory, Department of Chemistry, Dartmouth College,
     Hanover, NH, 03755, USA
SO   Organometallics (2005), 24(11), 2730-2746
     CODEN: ORGND7; ISSN: 0276-7333
PB   American Chemical Society
DT   Journal
LA   English
AB   The chiral Pd(0) trans-stilbene complexes Pd(diphos*)(trans-stilbene)
     (diphos* = (R,R)-Me-Duphos, (R,R)-Et-Duphos, (R,R)-i-Pr-Duphos,
     (R,R)-Me-BPE, (S,S)-Me-FerroLANE, (S,S)-Me-DuXantphos, (S,S)-Et-FerroTANE,
     (R,S)-CyPF-t-Bu, (R,S)-PPF-t-Bu, (R,S)-BoPhoz) and Ni((R,R)-Me-
     Duphos)(trans-stilbene) were prepared by NaBH(OMe)3 reduction of the
     corresponding M(diphos*)Cl2 compds. in the presence of trans-stilbene.
     The rate of oxidative addition of PhI to the stilbene complexes, which gave
     Pd(diphos*)(Ph)(I), depended on the ligand (larger for increased ligand
     bite angles and reduced steric bulk) and was markedly faster than
     oxidative addition to mixts. of Pd(dba)2 and diphos*. The complexes
     Pd(diphos*)(Ph)(I) were prepared independently by treatment of PdL2(Ph)(I)
     (L2 = TMEDA, (PPh3)2) with diphos*. Oxidative addition of PhI to the
     complexes M((R,R)-Me-Duphos)(trans-stilbene) occurred in the rate order Pd
     > Ni » Pt. The complexes Pd(diphos*)Cl2, Pd(diphos*)(trans-
     stilbene), and Pd(diphos*)(Ph)(I), as well as some analogous Ni compds.,
     were structurally characterized by x-ray crystallog.
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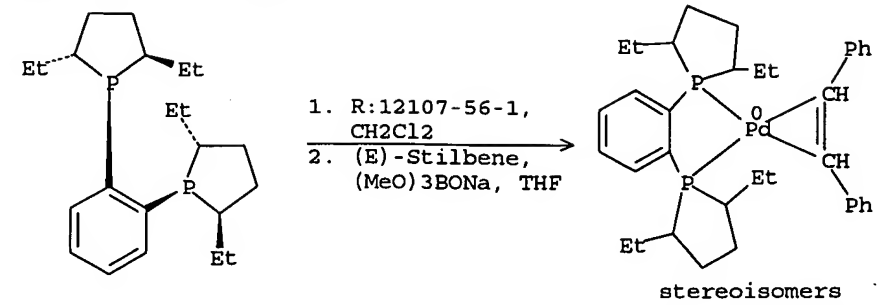
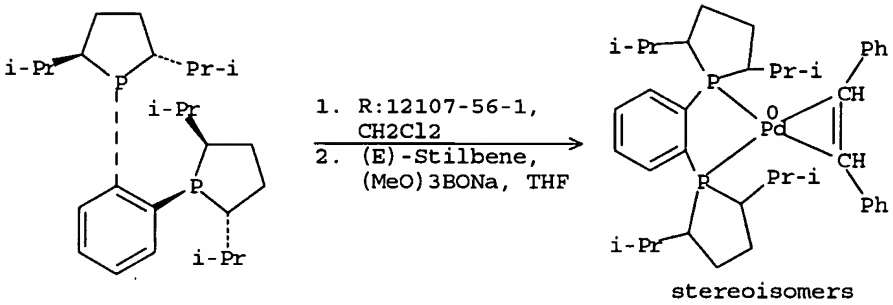
RX(51) OF 79 - 2 STEPS



stereoisomers

NOTE: 2) stereoselective, diastereomer ratio 7.8:1, 35% yield
CON: STEP(1) 1 hour, room temperature
STEP(2) 1 hour, room temperature

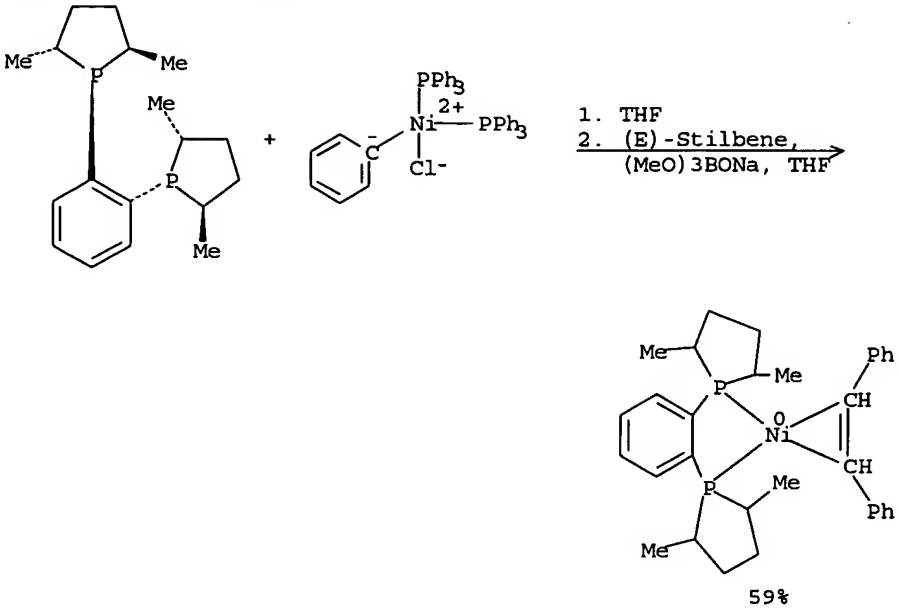
RX(52) OF 79 - 2 STEPS



stereoisomers

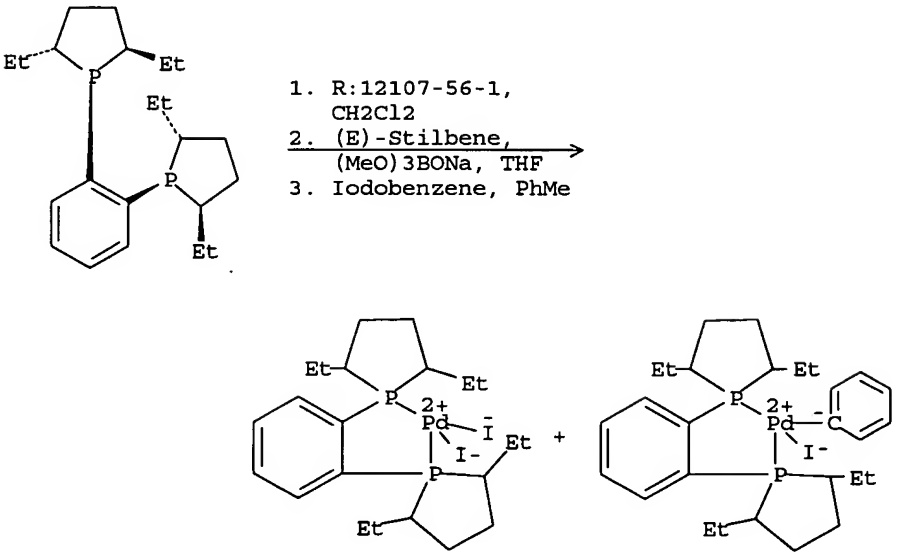
NOTE: 2) stereoselective, diastereomer ratio 38:1, 60% yield
CON: STEP(1) 1 hour, room temperature
STEP(2) 1 hour, room temperature

RX(70) OF 79 - 2 STEPS



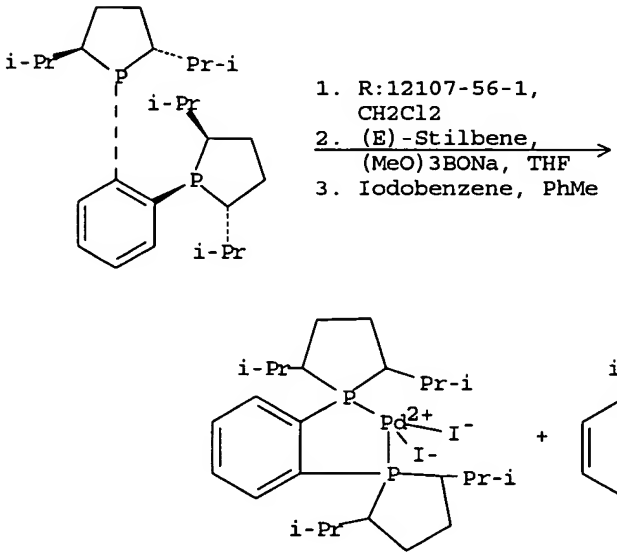
CON: STEP(1.1) 15 hours, room temperature
STEP(2) 1.5 hours, room temperature

RX(72) OF 79 - 3 STEPS



NOTE: 2) stereoselective, diastereomer ratio 7.8:1, 35% yield, 3)
NMR-scale experiment, product not isolated
CON: STEP(1) 1 hour, room temperature
STEP(2) 1 hour, room temperature
STEP(3) 3 hours, room temperature

RX(73) OF 79 - 3 STEPS



NOTE: 2) stereoselective, diastereomer ratio 38:1, 60% yield, 3)
NMR-scale experiment, product not isolated
CON: STEP(1) 1 hour, room temperature
STEP(2) 1 hour, room temperature
STEP(3) 9 hours, room temperature

RE.CNT 77 THERE ARE 77 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 15:41:52 ON 10 AUG 2006)

FILE 'HCAPLUS' ENTERED AT 15:41:58 ON 10 AUG 2006

L1	1	US2004167362/PN OR (US2003-670105 OR EP2002-256696)/AP,PRN
		E DRENT E/AU
L2	316	E3-6
		E GINKEL R/AU
L3	1	E4
		E VAN GINKEL R/AU
L4	13	E3,E9
		E JAGER W/AU
L5	83	E3,E9
		E JAGER WILLEM/AU
L6	38	E4-8
L7	4537	(SHELL OIL)/CS,PA

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     FILE 'REGISTRY' ENTERED AT 15:52:55 ON 10 AUG 2006

     FILE 'HCAPLUS' ENTERED AT 15:52:55 ON 10 AUG 2006
L8             TRA L1 1- RN :       17 TERMS

     FILE 'REGISTRY' ENTERED AT 15:52:55 ON 10 AUG 2006
L9            17 SEA L8
L10            6 L9 AND P/ELS
L11              STR
L12            5 L11
L13          179 L11 FULL
                 SAV TEM LAO105/A L13
L14            4 L13 AND L9

     FILE 'HCAPLUS' ENTERED AT 15:57:52 ON 10 AUG 2006
L15          290 L13
                 E ALKENES/CT
L16       197017 E3+OLD,NT (L) RACT+NT/RL
                 E E3+ALL
                 E ALKENES,/CT
L17        26487 ALKENES/CW (L)RACT+NT/RL
L18           87 L16-17 AND L15
                 E LIGANDS/CT
                 E E3+ALL
L19           33 E1+NT (L) BIDENTAT? (L)DIPHOSPH?
L20           10 L16-17 AND L19
L21           96 L18,L20
                 E HYDROFORMYLATION/CT
L22         2889 E3-9
L23         2889 E3+OLD,NT
                 E E12
                 E E3+ALL
L24         4610 E4+OLD
                 E HYDROFORMYLATION ENTHALPY/CT
L25            7 E3+OLD,NT
L26          416 HYDROFORMYLATION KINETICS+OLD,NT/CT
L27           18 L21 AND L22-26
L28            4 L27 AND L1-7
L29           14 L27 NOT L28
                 E GROUP VIII ELEMENTS/CT
                 E E3+ALL
L30            5 E6+NT AND L27
L31           13 E69+OLD,NT AND L27
L32           15 L30-31
L33            3 L32 AND L1-7
L34           12 L32 NOT L33
                 E CATALYSTS/CT
L35         4443 E3+OLD,NT (L) HYDROFORMYL?
L36           18 L35 AND L21
L37            0 L36 NOT L27
L38            5 L34 AND (PY<=2002 OR AY<=2002 OR PRY<=2002)
L39           12 L34,L38

     FILE 'CASREACT' ENTERED AT 16:12:39 ON 10 AUG 2006
L40              STR L11
L41            0 L40
L42            1 L40 FULL

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